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Scientific Notebook No. 532E: In-Drift Thermal Radiation and Forced Ventilation Model (DRIFTVNT) Vol. 1: Ventilation Model, Vol. 2: Edge Effects, Vol. 3: Surface Temperature, and Vol. 4:Code Analysis (07/18/2002 through 11/13/2003)

SCIENTIFIC NOTEBOOK

by

George Adams

SCIENTIFIC NOTEBOOK No. 532E-Vol 1(Ventilation Model)

SCIENTIFIC NOTEBOOK

by

George Adams

Southwest Research Institute Center for Nuclear Waste Regulatory Analyses San Antonio, Texas

SCIENTIFIC NOTEBOOK No. 532E-Vol 1(Ventilation Model)

INITIAL ENTRIES

Scientific Notebook: #532E

Issued to: G. Adams

Issue Date: July 18, 2002

Account Number: 20-5708-661

Title: DRIFTVNT

Participants: George Adams,

Scott Painter

July 19, 2002, GADAMS:

The objectives of this task are in accordance with the Software Requirements Description for the Computer Code DRIFTVNT. The objective of this task is to implement the In-Drift Thermal Radiation and Forced Ventilation Model referenced in the software requirements description document.

The approach to achieving the objectives will be to develop an interface module and a main module. The interface module will retrieve configuration parameters from an input file and transform cell by cell information into slice by slice information. The main module will process slice by slice information.

The qualifications for performing this task are proficiency in developing, implementing, and testing FORTRAN 77 code.

For this coding effort, multiflo version 1.5 code will be retrieved from machine spock. This code will be maintained as a baseline code version. A copy of the baseline code version will be edited to interface to the DRIFTVNT interface module. The DRIFTVNT modules will be maintained separately from the multiflo code. The DRIFTVNT modules built under this task will become a baseline version for configuration management purposes.

Software development and testing will be performed on machine spock. This machine is a SUN Ultra-4 server with Solaris 5.8. Source code will be placed and software development will be performed under the directory \$HOME/tefbuild. Software will be built using the FORTRAN 77

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compiler on this machine.

An incorrect account number was previously entered. The correct account number is 20.01402.661.

August 8, 2002, GADAMS:

The reference used in this development effort which will be incorporated into the validation testing of the code module is the following:

Painter, S., C. Manepally, and D.L. Hughson. "Evaluation of U.S. Department of Energy Thermohydrologic Data and Modeling Status Report." San Antonio, Texas: CNWRA. September 2001.

In-Process Entries

August 15, 2002, GADAMS:

The code module mysrc.f was separated into three separate code modules: idrift.f, drift.f, and driftvnt.h. In addition, a data file, driftvnt.dat was added. Three changes were incorporated into the initial build. The first two changes involved formating GADAMS 8-15-02 formatting and indexing changes into the source array is. The third change involved adding sources that were not located at the emplacement drift surface. The third change also incorporated a configurable slice length. Change 3 was built and tested against a baseline build. For the baseline, the output file is heatload. For the updated code modules the output file is driftvnt.out. Test 1 involved running the driver for driftvnt and verifying the output files were the same as the base case. Test 2 involved running the integrated driftvnt code and verifying the output files were the same as the base case. For the integrated test, a single time step was used. Test 3 was a test similar to Test 2 except the emissivity was set to 0. For both tests 1 and 2, the output files corresponded to those from the base case. Build and test results are included on ZIP disk: SN532E-VOL1:DISK1. The baseline build and test is included in archive: SPOCKHOMEtefbuildbaseline. The updated files for changes 1 through 3 are included in archive: SPOCKHOMEtefbuildbuildchange1, SPOCKHOMEtefbuildchange2, and SPOCKHOMEtefbuildchange3. The tests for change 3 are included in archive: SPOCKHOMEtefbuildtestTEST8-15-02. All building of code modules and testing were performed on machine spock.

August 20, 2002, GADAMS:

Discovered an error in change 3 of the code in which the radfac variable was not calculated correctly. In addition, end effects were added to the model. The end effects were considered an additional number of sources sent to the idrift module. An additional change was made in which the number of sources which is passed as a parameter is checked against the number of sources

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dr GADAMS 8-20-02 derived from driftvnt.dat. If the number of sources do not match, then the driftvnt code stops and generates an error messages. The code was rebuk GADAMS 8-20-02 rebuilt and tested on machine spock. Updated files and test results are included on ZIP disk: SN532E-VOL1:Disk1. The updated files are included in archive SPOCKHOMEtefbuildbuildchange4. The test results are included in archive: SPOCKHOMEtefbuildtestTEST8-20-02. From test2, the test2.out file and the base.out file from the baseline tests conduce GADAMS 8-20-02 conducted previously were compared. Since the error in radfac was corrected, these two files showed the same metra results.

Entries into Scientific Notebook #532E-Vol1 for pages \ \ - \ \ have been made by George Adams 8/23/04.

No original text entered into this Scientific Notebook has been removed.

Ning Q John 8/23/04

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

Hordon Witheneye 9/21/2004

SCIENTIFIC NOTEBOOK

by

George Adams

SCIENTIFIC NOTEBOOK No. 532E-Vol 2(Edge Effects)

SCIENTIFIC NOTEBOOK

by

George Adams

Southwest Research Institute Center for Nuclear Waste Regulatory Analyses San Antonio, Texas

SCIENTIFIC NOTEBOOK No. 532E-Vol 2(Edge Effects)

INITIAL ENTRIES

Scientific Notebook: #532E

Issued to: G. Adams

Issue Date: July 18, 2002

Account Number: 20-01402-661

Title: CONDRIVE (Analyze Edge Effects in the Repository)

Participants: George Adams,

Randy Fedors (Scientific Notebook 432E-VolVIII)

August 8, 2002, GADAMS:

The objective of this task is to develop a driver for the condxyzt module. The driver will be named CONDRIVE. This driver will allow the condxyzt module to run standalone.

The approach to achieving this objective is to develop the CONDRIVE module, include an input file for initialization and configuration parameters, include a call to the cond3dxyzt subroutine, and generate output to the screen.

The qualifications for performing this task are proficiency in developing, implementing, and testing FORTRAN 77 code.

The current version of the TPA code is Version 4.2h. The following modules were GADAMS 8-8-02 retrieved from this code version: array.f, condxyzt.f, fileunit.f, invent.f, numrecip.f, and zportunx.f.

Software development and testing will be performed on machine spock. This machine is a SUN Ultra-4 server with Solaris 5.8. Source code will be placed and software development will be performed under the directory \$HOME/condxyzt. Software will be built using the FORTRAN 77 compiler on this machine.

In-Process Entries

August 9, 2002, GADAMS:

Built the driver for the condxyzt module. The driver file is condrive.f. The code modules used in this development effort were for version 4.2i of the TPA code instead of version 4.2h. The condrive module has a configuration and input file titled "condrive.dat." In order to set configuration parameters, the following was performed: 1) The TPA code was executed for 1 realization and 1 subarea (subarea 1). 2) The mean tpa input file "tpameans.out," was used as the new tpa.inp file. 3) The TPA code was executed for this mean case and the parameters in mv.tpa and tpa.inp were used as configuration parameters in condrive.dat. The following table summarizes these configuration parameters.

Name	Reference	Value
rhoin	MassDensityofU GADAMS 8-9-02 MassDensityofYMRock	2580.0
Cpin	SpecificHeatofYMRock	840.0
Condin	ThermalConductivityofYMRock	1.56
amlin	DriftArealMassLoading	926.07
bftimein	TimeOfBackfillEmplaced	50.0
hloss_factin	FactorForVentilationHeatlosses	0.7
npoints	npoints NumberOfWeightsForGaussLegendreIntegration	
num_drifts	m_drifts NumberOfDriftsInrepository	
drift_dia	drift_dia EmplacementDriftDiameter	
elevation		

Verification of the driver was performed in the following way: 1) Code module nfenv.f from the TPA 4.2i distribution was modified to print out the coordinates used in its calculations along with the drift associated with these coordinates. 2) The updated TPA code was executed for the mean case, 1 realization and subarea 1. The TPA.inp file was modified to set AmbientRepositoryTemperature to 0. The output from the TPA run, file nfenv.rlt was generated. 3) The driver was executed at two time steps. One time step was 1900 years and the second time

step was 10,000 years. 4) The output from the driver and the TPA code was compared. The following table summarizes the comparison of results.

Target	Result(1900 years)	Result(10,000 years)
X = 547695.17313185 Y=4078529.0951943	Point 835 of 1000 X = 547695.53998709	Point 835 of 1000 X=547695.53998709
Drift 9	Y=4078528.9801021 Temp = 70.228223	Y=4078528.9801021 Temp=32.957938
Time = 1900, temprep =	. •	•
70.208	Point 836 of 1000	Point 836 of 1000
	X=547694.66568959	X=547694.66568959
Time = 10,000, temprep =	Y=4078529.2543924	Y=4078529.2543924
32.949	Temp = 70.182606	Temp=32.937864

The above table shows that the output temperatures at the desired point in drift 9 correspond to the expected(target) temperatures at the times of 1900 years and 10000 years. This verification test shows that the driver produces the results expected from the TPA code. Output and supporting files are included on ZIP disk SN532E-VOL2:DISK1. The rebuild of the TPA code with the updated nfenv.f module is included under directory SPOCKHOMETEST8-9-02condver. The verification files are included under directory SPOCKHOMETEST8-9-02verification.

August 15, 2002, GADAMS:

Updated the condrive.f code module to accept an array of time values so that the simulation can be run over this array of values. Also, there was an error in the original code in which the endpoints of the drift were not moved outside of the drift coordinates but were instead moved inside. This error was corrected. The new code was rebuilt on machine spock in the following directory: \$HOME/condxyzt/build2. The code was retested and verified at two time points against the previous TPA code results generated in file nfenv.rlt. Within condrive.out, the following information was obtained:

```
723 5.47696196E+05 4.07852877E+06 70.26 32.97
```

These points correspond to the data obtained at time = 1900 and time = 10000 years in nfenv.rlt which is listed as follows:

```
131 1.9000E+03 7.0208E+01
```

The required coordinates were X=547695 and Y=4078529. Therefore the values obtained from condrive correspond to those expected from the TPA code.

The build and test results are included on ZIP disk SN532E-VOL2:DISK1. The build is in

^{724 5.47694884}E+05 4.07852919E+06 70.19 32.94

^{201 1.0000}E+04 3.2949E+01

archive: SPOCKHOMEcondxyztbuild2 and the tests are in archive: SPOCKHOMEcondxyztrunTEST8-15-02.

October 21, 2002, GADAMS:

Updated the code module condrive.f to accept the ambient temperature of the repository as an input parameter in condrive.dat. In addition, rebuilt the condrive module to use the associated 4.1j TPA code modules. The new build is located on ZIP disk SN532E-VOL2:DISK1 in archive: SPOCKHOMEcondxyztbuild3.

October 22, 2002, GADAMS:

Rebuilt TPA code version 4.1j with one modification to module NFENV.F. The NFENV> GADAMS 10-22-02 NFENV.F module was modified to include 3 print statements to print out the drift at the center of the subarea and the x,y coordinates at the center. This change was done to perform verification testing of the condrive module against the TPA code. This modified TPA 4.1j code version is located on ZIP disk SN532E-VOL2:DISK1 in archive: SPOCKHOMEcondxyztcode41j_mod.

Performed verification testing of the condrive modue GADAMS 10-22-02 module against the modified TPA 4.1j code. The following table summarizes the test output: Drift 33, point 72 was selected because it is close to the center point used in the TPA code. The TPA coordinates for subarea 1's center point are: 547695.17313185, 4078529.0951943. The condrive coordinates for point 72 are: 5.47699059E+05, 4.07853315E+06. The results for the

NFEN	CONDRIVE.OUT	
TIME	TEMPREP	TEMPERATURE (POINT 72)
0	23.35	23.35
1900	80.608	80.50(time=1976)
10000	48.73	49.04(time=9989)

time=1900 row of the above table differ by 0.13%. The results for the time=10000 row of the above table differ by 0.64%. The test results are located on ZIP disk SN532E-VOL2:DISK1 in archive: SPOCKHOMEcondxyztrunTEST10-21-02.

December 19, 2002, GADAMS:

A new build, build 4, was created for the condrive module. This build incorporates the following changes: 1) Added the path include file, path.i, to the condrive module, condrive.f. This change allows the driver to retrieve the drifts.dat and condrive.dat files from the data directory specified by the environment variables. 2) Added property 2 data. At a position distance_east in meters

from the East end of a drift, the user has the option to use property 2 data. 3) Added header information to condrive.out (Date/Time). Also, modified the code to delete any previously existing condrive.out file on startup.

Two tests were conducted on this new build. These tests are described as follows:

- 1) Test 1 compares the build 4 output with the build 3 output. The distance from the East end of the drift is set to 0 in condrive.dat. For this test case, both builds generate the same output results as expected. Note: build 4 generates a header in the output file. This header contains the date and time of the run.
- 2) Test 2 takes an input distance from the East end of the drift, identifies which of the points should use property 2 data, and verifies the condrive module identifies those points which should use property 2 data. An input distance of 4 meters was used and the first 9 points use the property 2 data as expected.

Build and test results are located on ZIP disk SN532E-VOL2:DISK1 in archive SPOCKHOMEcondxyztbuild4.zip.

March 12, 2003, GADAMS:

Created a new build, build5, for the condrive module. This build incorporates the following changes: 1) Modified the drifts.dat file to include the x-coordinate locations where the repository changes to TSW34, TSW35, and TSW36. 2) Modified the condrive module to consider three possible types of areas containing heat sources in each drift. The three possible area types are: TSW34, TSW35, and TSW36.

Two types of verification tests (Test 1 and Test 2) were conducted. Test 1 consisted of four test cases (A through D). Test 2 consisted of six test cases (A through F). Test 1 was designed to compare the build5 code to the build3 code. The results for Test 1 showed that the temperature changed as expected for transitions among TSW34, TSW35, and TSW36. Test 2 was designed to analyze the temperature difference between the center and the edge of the drift for three different sets of thermal conductivities and two different drifts. Drift 25 passes through TSW34 and TSW35 and shows the increase in temperature difference for the rise in thermal conductivity from the center to the edge of the drift. In addition, the transitions from wet to average to dry thermal conductivities, (and the corresponding drop in thermal conductivity for each transition), appear as greater overall temperature differences from center to edge of drift as expected. Drift 49 was also analyzed. It passes through TSW34, TSW35, and TSW36. The transitions that were apparent for drift 25 between TSW34 and TSW35 are not apparent in the plots for drift 49. A much smaller amount of TSW34 is present in drift 49 compared to drift 25.

Build and test results are located on ZIP disk SN532E-VOL2:DISK1 in archive

SPOCKHOMEcondxyztbuild5.zip.

March 24, 2003, GADAMS:

A module was modified to extract temperature gradients from the condrive output file. This module is named drift.f. The module is used to extract the following gradients:

1) The temperature difference calculated using the temperature at the center.

[T(center) - T(i)], where i = 1, n; i = 1 is the center and i = n is the edge.

2) The temperature gradient calculated using the temperature at the center.

[T(center) - T(i)] / L(i), where L(i) is the absolute GADAMS 3-24-03 distance from the center to the location of temperature T(i).

3) The local temperature gradient calculated from adjacent points.

[T(i) - T(i+1)] / [x(i+1) - x(i)], where T(i) is closer to the center.

The above modification was identified as modification3-17-03. However, when plots for the East end of drifts 25 and 49 were generated, the negative distances caused the temperature gradients to flip about the x-axis. Therefore, the code was modified from 3-17-03 to use the absolute value of the distance for 2 above and the absolute value of the difference for 3 above. This modification was identified as modification3-24-03.

A series of plots were generated using the condrive build5 module and the updated drift module. These were plots for the temperature profiles in drift 25 and drift 49. In addition to the temperature profiles, temperature gradients in these drifts were plotted. In order to generate these plots, the following information was used: (condrive.out files from)

Drift 25 East and West Average Thermal Conductivity Plots:

condxyzt\build5\verification\test2\testB

Drift 25 East and West Wet Thermal Conductivity Plots:

condxyzt\build5\verification\test2\testC

Drift 49 East and West Average Thermal Conductivity Plots:

condxyzt\build5\verification\test2\testE

Drift 49 East and West Wet Thermal Conductivity Plots:

condxyzt\build5\verification\test2\testF

The drift module is located on ZIP disk SN532E-VOL2:DISK1 in directory GADAMS 3-24-03 archive SPOCKHOMEcondxyztgradient.zip. The plots are located on ZIP disk SN532E-VOL2:DISK1 in archive SPOCKHOMEcondxyzttemperaturegradientplots.zip.

April 23, 2003 GADAMS:

An analysis was performed on the drift module to verify the values it generated. Hand calculations were performed at three points generated by the condrive module at four different temperatures. The values from condrivewetdrift25east.xls included in archive

SPOCKHOMEcondxyzttemperaturegradientplots.zip from the previous entry were used in this analysis. A summary of the calculations is shown in the following table (the notation in the table is hand calculated/drift module generated):

Point ***	Distance	Peak Peak	T100	T80 4 4 4	Tend
84	. =	73/73	57.73/57.73	48.67/48.67	38.55/38.55
310	-	138.5/138.5	93.12/93.12	69.2/69.2	48.22/48.22
400	· <u>-</u>	139.09/139.09	97.47/97.47	72.65/72.65	49.8/49.8
Point 1	Distance	Diff Peak 444	Diff100	Diff80 d	Diffend
84		66.06/66.06	41.23/41.23	25.39/25.39	11.85/11.85
310	-	0.56/0.56	5.84/5.84	4.86/4.86	2.18/2.18
400	-	-0.03/-0.03	1.49/1.49	1.41/1.41	0.6/0.6
Point	Distance	GradPeak	. Grad100	Grad80	Gradend
84	557.723	0.1184/0.11845	0.0739/0.073926	0.0455/0.045524	0.0212/0.021247
310	255.093	0.0022/0.0022	0.0229/0.022894	0.0191/0.019052	0.0085/0.0085459
400	134.577	-0.0002/-0.0002	0.0111/0.011072	0.0105/0.010477	0.0045/0.0044584
Point :	Distance	LocGradPeak	LoeGrad100	LocGrad80	LocGradend
84	557.723	5.1755/5.1743	0.3361/0.336	0.1344/0.1344	0.0523/0.052266
83	559.062		1.		
310	255.093	0.0448/0.0448	0.0597/0.059733	0.0448/0.0448	0.0149/0.014933
309	256.432		;		
400	134.577	0/0	0.0224/0.0224	0.0224/0.0224	0.0075/0.0074666
399	135.916				

April 29, 2003 GADAMS:

Created a series of plots to show the significant temperature gradient, both a local temperature gradient and an overall temperature gradient.

In order to generate this information, the drift.f script was modified to generate significant gradient information. An input file, drift.dat, sets the threshold for the drift code to be used in determining whether or not a gradient is significant. The new version of the drift module is located on ZIP disk SN532E-VOL2:DISK1 in archive SPOCKHOMEcondxyztgradientmodification4-24-03.zip.

- 1) For the overall gradient, first an initial point from the edge is found if its temperature difference from the center is above the threshold and if its temperature difference from the edge is above the threshold. (Note: In all cases, the absolute value of the difference is used.) Next, the last point going from the edge to the center for which the temperature difference between that point and the center exceeds the gradient is determined. Once these two points along the half-drift are found, the distance between them is the length of the half-drift having a significant overall temperature gradient. This length is divided by the length of the half-drift to generate the fraction of the half-drift having a significant overall temperature gradient.
- 2) For the local gradient, the number of local gradients along the half-drift for which their temperature per unit length is above the threshold is counted. Then, this sum is divided by the total number of gradients along the half-drift. This value is the fraction of all local gradients along the half-drift having a significant local temperature gradient.

A total of 8 plots were generated and included in the following Excel spreadsheets: condriveavgdrift25east.xls, condriveavgdrift25east.xls, condriveavgdrift25west.xls, condriveavgdrift49east.xls, condriveavgdrift49east.xls, condriveavgdrift49east.xls, and condrivewetdrift49west.xls.

The plots are located on ZIP disk SN532E-VOL2:DISK1 in archive SPOCKHOMEcondxyzttemperaturegradientplots4-24-03.zip.

April 29, 2003 GADAMS:

Conducted a verification test of the drift module for the changes identified in the previous entry. Calculations were performed for both the local gradient and the overall gradient at different times and thresholds. Calculations in an Excel Spreadsheet compared well with the output generated by the drift module. The following table summarizes the results of the calculations and the output generated by the module. (Calculations were performed for the East end of Drift 25 with average thermal conductivities.)

Time	Threshold	Overall Gradient	Drift Module Output
973.5	1.0	0.774038	0.77404
53.9	0.5	0.526439	0.52644
9988.6	0.25	0.877401	0.8774
Time)	Threshold	Local Gradient	Drift Module Output
84	0.1	0.1942446	0.19424
6976.2	0.05	0.2110312	0.21103

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1075	0.025	0.729016	0.72902
20,0		0.7.25010	0.72702

The calculations are included on ZIP disk SN532E-VOL2:DISK1 in archive verificationgradient4-24-03.zip.

October 17, 2003 GADAMS:

An update to the test conducted under entry April 29, 2003 GADAMS contained in archive SPOCKHOMEcondxyzttemperaturegradientplots4-24-03.zip was conducted. An additional test for drift 25 was conducted on machine SPOCK for the East and West ends of the drift wet and average thermal conductivities. For this additional test, the temperature gradients were calculated for an overall threshold of 5 C and a local threshold of 0.5 C/m.

The test results are located on ZIP disk SN532E-VOL2:DISK2 in archive: SPOCKHOMEcondxyzttemperaturegradientplots10-16-03.zip.

Entries into Scientific Notebook #532E-Vol2 for pages _\ _ - _\\ have been made by George Adams 8/23/04.

No original text entered into this Scientific Notebook has been removed.

Bug & Mary 8/23/04.

Godor Wittnessen

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

SCIENTIFIC NOTEBOOK

by

George Adams

SCIENTIFIC NOTEBOOK No. 532E-Vol 3(Surface Temperature)

SCIENTIFIC NOTEBOOK

by

George Adams

Southwest Research Institute Center for Nuclear Waste Regulatory Analyses San Antonio, Texas

SCIENTIFIC NOTEBOOK No. 532E-Vol 3(Surface Temperature)

INITIAL ENTRIES

Scientific Notebook: #532E

Issued to: G. Adams

Issue Date: July 18, 2002

Account Number: 20-06002-01-091

Title: TEMPSURF (Analyze the waste package surface temperature.)

Participants: George Adams,

Chandrika Manepally (Scientific Notebook 478E-Vol5)

February 7, 2003 GADAMS:

The objective of this task is to develop a standalone module to analyze the waste package surface temperature. The module will be named TEMPSURF.

The approach to achieving this objective is to develop the TEMPSURF module, include input file(s) for initialization and configuration parameters, and generate output to the screen.

The qualifications for performing this task are proficiency in developing, implementing, and testing FORTRAN 77 code.

Software development and testing will be performed on machine spock. This machine is a SUN Ultra-4 server with Solaris 5.8. Source code will be placed and software development will be performed under the directory \$HOME/tempsurf. Software will be built using the FORTRAN 77 compiler on this machine.

SCIENTIFIC NOTEBOOK No. 532E-Vol 3(Surface Temperature)

In-Process Entries

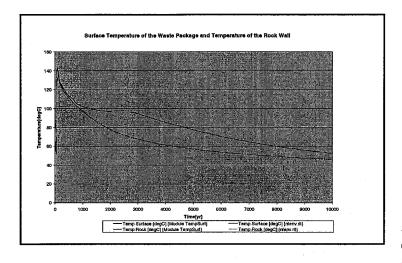
May 6, 2003 GADAMS:

Build 1 of the TempSurf module was built and tested. This module calculates the waste package surface temperature using equations taken from tpa4.1j. Modifications made include the following:

- 1) Thermal input versus time and rock wall temperature versus time are retrieved from an input data file, tempsurf.dat. The thermal input is interpolated to the time-rock wall temperature time steps and is then used directly to calculate the temperature of the waste package (A heat loss factor is not subtracted for the preclosure period).
- 2) Equation 5-11 from the Total-System Performance Assessment (TPA) Version 4.0 Code: Module Descriptions and User's Guide, November 2000 was modified. The tpa4.1j code includes the term condbf in the numerator which is the effective thermal conductivity of the backfill material. This term was removed from the TempSurf code. In addition, the drip shield outer diameter was calculated as the sum of the drip shield inner diameter and the drip shield thickness in the tpa4.1j code. In TempSurf, the drip shield outer diameter is instead calculated as the sum of the drip shield inner diameter and twice the sum of GADAMS 5-6-2003 the drip shield thickness.
- 3) Equations 5-6 and 5-7 from the TPA Version 4.0 Code: Module Descriptions and User's Guide were also modified. The middle term in the denominator for these two equations does not include waste package spacing. In TempSurf, waste package spacing was added to this middle term.

In addition to performing hand calculations of the TempSurf output, a comparison was done on the tpa4.1j code for a mean value tpa.inp case on one subarea and one realization over 10,000 years. The waste package surface temperature versus time was plotted for this tpa4.1j case, and the waste package surface temperature versus time was plotted for the TempSurf code output. This plot is shown below:

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An additional comparison was conducted in the

tpa4.1j code using tabulated temperature-relative humidity data. The file, tefkti.inp, was used and the tabulated temperature and relative humidity were read for the four data sets in the file. The four data sets appear to contain the same data in the tpa4.1j code.

For this testing, the TempSurf code and the tpa4.1j code was built on machine spock. The code and test results are include on A GADAMS 5-6-2003 ZIP disk: SN532E-VOL3DISK1 in archive: SPOCKHOMEtempsurfbuild1.

Entries into Scientific Notebook #532E-Vol3 for pages _ \ _ - \ _ have been made by George Adams 8/23/04.

No original text entered into this Scientific Notebook has been removed.

Dung & Many 8/23/04

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

Godan Withneye 9/21/2004

SCIENTIFIC NOTEBOOK No. 532E-Vol 3(Surface Temperature)

SCIENTIFIC NOTEBOOK

by

George Adams

SCIENTIFIC NOTEBOOK No. 532E-Vol 4(Code Analysis)

SCIENTIFIC NOTEBOOK

by

George Adams

Southwest Research Institute Center for Nuclear Waste Regulatory Analyses San Antonio, Texas

SCIENTIFIC NOTEBOOK No. 532E-Vol 4(Code Analysis)

INITIAL ENTRIES

Scientific Notebook: #532E

Issued to: G. Adams

Issue Date: July 18, 2002

Account Number: 20-06002-01-091

Title: Code Analysis (Analyze the code in terms of models and/or documentation.)

Participants: George Adams,

Chandrika Manepally (#478E),

Steve Green (#536E), Randy Fedors (#432E)

April 8, 2003 GADAMS:

The objective of this task is to analyze the code in terms of models and/or available documentation.

The approach to achieving this objective is to use baseline versions of the TPA code (4.1j) and verify the information generated by the code. Modifications will be made as necessary to generate output information for analysis.

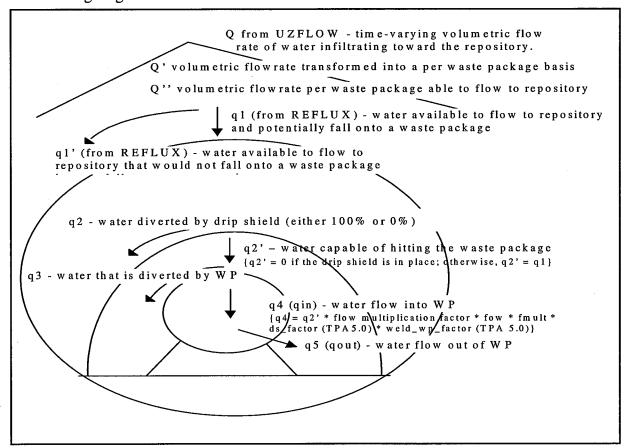
The qualifications for performing this task are proficiency in developing, implementing, and testing FORTRAN 77 code.

Software development and testing will be performed on machine spock. This machine is a SUN Ultra-4 server with Solaris 5.8. Source code will be placed and software development will be performed under the directory \$HOME/tpabuild_study. Software will be built using the FORTRAN 77 compiler on this machine.

In-Process Entries

April 10, 2003 GADAMS:

The following entry is a flowrate analysis on the TPA code. A summary of the flows is shown in the following diagram.



A discussion of the individual terms shown in the diagram are included as follows:

Equation 1:

Q' (m^3 / (yr-wp)) = Q {the amount of water infiltrating the ground surface in a subarea in a given year, m^3/yr } / (The Number of Waste Packages in that Subarea) Q" (m^3 / (yr-wp)) = the amount of Q' able to flow to a drift in the repository.

Equation 2:

$$Q'' = q1 + q1'$$

where,

q1 = that portion of Q" that is available to flow to a waste package in the repository q1' = that portion of Q" that is available to flow to the repository but would not hit a waste package

Equation 3:

q2' = 0, if the current time is less than the drip shield failure time q2' = q1, if the current time is greater than or equal to the drip shield failure time

q2 = q1 - q2' {not implemented in the code}

Equation 4:

q4 = q2' * flow multiplication factor * fmult * fow * ds_factor(TPA5.0) * weld_wp_factor(TPA5.0), if the number of waste package failures is greater than 0

q4 is not calculated if there are no waste package failures

q3 is not implemented in the code

Equation 5:

q5 = q4 for the flowthrough model

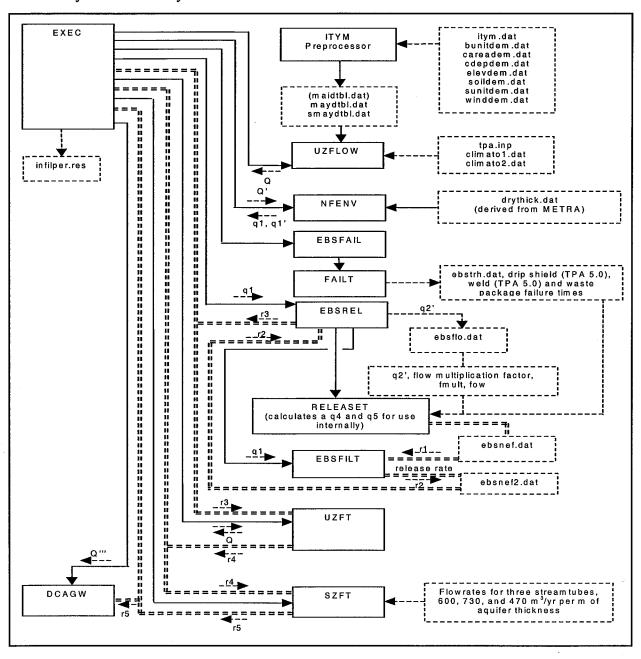
q5 = q4, if the waste package is full under the bathtub model q5 = 0, if the waste package is not yet full under the bathtub model

Equation 6:

Q" = the average Q for each time interval divided by the number of years in that time interval, summed over TPA time intervals and averaged for the entire TPA analysis period.

Q''' = sum over TPA time intervals ((Q[I] - Q[I-1]) / (time[I] - time[I-1])) / analysis period

A summary of the flows by modules in the TPA code is included as follows:



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April 14, 2003 GADAMS:

A series of module level descriptions associated with the previous two figures included in entry April 10, 2003 GADAMS are included below:

EXEC:

- 1. Retrieves Q from UZFLOW, converts the flux to Q', the amount of water infiltrating the ground surface in a given year per waste package (m^3/yr-wp) and then invokes NFENV passing Q' to this subroutine.
- 2. Retrieves q1 from NFENV and invokes EBSREL passing q1 to EBSREL.
- 3. Generates output file infilper.res using Q, q1, fmult, fow, and the waste package flow multiplication factor. A sample of infilper.res follows: UZFLOW:

	•	Wed Jan 22 15:3 tion/Deep Percolat		
After Reflu	x and Diversion	n - Values for Eac	h Vector	fow: 0.173205 fmult: 0.044721
vector	time	avinfil	avreflux	wpflow: 1.984585
avdivert				avdivert = 6.9754 * 0.173205
unitless	yr	mm/yr	mm/yr	* 0.044721 * 1.984585
mm/yr 1 0.0000E+00	0.0000E+00	1.4938E+01	0.0000E+00	therefore avdivert = 0.107229
1	2.5694E+01	1.4938E+01	1.0643E+01	
1.6361E-01				
1 1.0723E-01	5.8078E+01	1.4938E+01	6.9754E+00	

1. Calculates Q, the amount of water infiltrating the ground surface in a given year (m³/yr).

NFENV:

Using one of 3 reflux models, takes as input Q', and

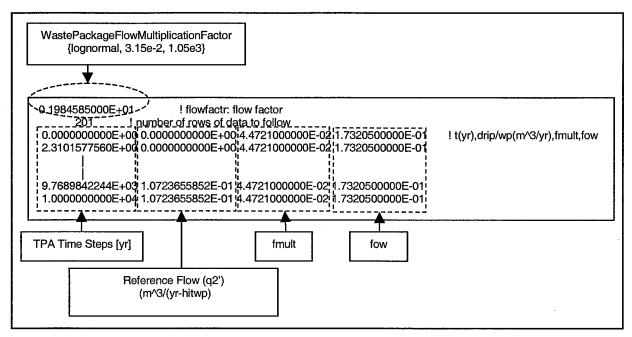
- 1. Calculates Q", the amount of Q' available to flow to the repository.
- 2. Calculates q1, that portion of Q" that is available to flow to a waste package in the repository.

3. Calculates q1', that portion of Q" that is available to flow to the repository but would not hit a waste package.

EBSREL

Retrieves q1 from EXEC and builds the input file ebsflo.dat as follows:

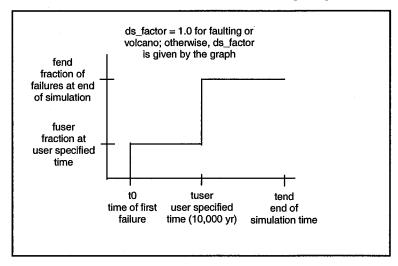
- 1. Builds a value q2' (Reference Flowrate), the flux capable of hitting a waste package by the following:
- a. For times at or after the drip shield failure time, transfers q1 to ebsflo.dat.
- b. For times below the drip shield failure time, transfers a value of 0 in place of q1 to ebsflo.dat.
- 2. Retrieves a waste package flow multiplication factor
- (WastePackageFlowMultiplicationFactor) from TPA.INP. This factor accounts for the flow loading (flowfactr: reference releaset.f) in a subarea and is defined as a lognormal distribution {3.15e-2, 1.05e3}.
- 3. Generates values for two additional factors, fmult (reference: wpflow.def, flow diversion) and fow(reference: wpflow.def, flow contacting waste packages, reference: releaset.f, fraction of water getting into the waste package), as follows:
- a. Using the file wpflow.def interpolates a set of predefined fmult and fow factors to TPA time steps. Currently, fmult and fow are constant over all time steps. Places these values interpolated to TPA time steps in file wpflow.dat.
- b. Retrieves the fmult and fow factors from wpflow.dat and places them in file ebsflo.dat. A sample of ebsflo.dat follows:



RELEASET:

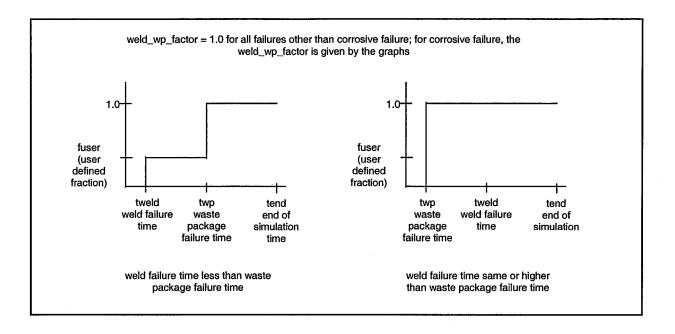
1. Invoked by EBSREL and computes a flowrate into the waste package, q4 (reference: releaset.f, qin). The flowrate into the waste package is the product of the flow multiplication factor, fmult, fow, ds_factor (TPA5.0), and weld_wp_factor (TPA5.0). (Note: The factor, ds_factor, is determined by the failure mechanism and the drip shield failure time. The factor, weld_wp_factor, is determined by the failure mechanism, the weld failure time, and the waste package failure time.)

2. The ds_factor is described in the following diagram:



3. The weld_wp_factor is

described in the following diagram:



4. Invoked by EBSREL and computes a release out of the waste package corresponding to a flowrate out, q5, (reference: releaset.f, qout) if there is a positive number of waste package failures; otherwise, no release (or flowrate out) is calculated.

EBSFILT:

1. Invoked by EBSREL. Takes the release rate from RELEASET and filters it through a transfer function that approximates transport through the concrete invert.

April 15, 2003 GADAMS:

A flowrate analysis was conducted using version 4.1j of the TPA code. The code was run for one realization on subarea 1. Test results are located on ZIP disk SN532E-VOL4:DISK1 in archive SPOCKHOMEtpabuild_studytpa41jmodrunTEST4-8-03. The following is a summary of the flowrate analysis:

The following analysis was conducted using TPA4.1j for 1 realization on subarea 1:

Subarea 1:

Number of waste packages: 1455

Q taken from uzflow.rlt.

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Q' calculated using information in uzflow.rlt and the number of waste packages in subarea 1 printed to the screen.

Q" modified nfenv.f to generate (Q" * number of waste packages) in file reflux3.out.

q1, q1' taken from nfenv.rlt.

{q1} calculated using waste package length (WPLength[m] tpa.inp4.1j) equal to 5.275 m and waste package diameter (WPDiameter[m] tpa.inp4.1j) equal to 1.579 m and the area of the subarea printed to the screen (723591.3 m²).

Fraction that hits a single waste package = ((5.275 * 1.579) / (723591.3) = 1.1511e-5

 $\{q1'\}$ calculated by taking $\{Q'\} - \{q1\}$

Time [yr]	Q [m^3/yr]	{Q'}	Q" * numwp	q1	{q1}	q1'	{q1'}
		[m^3/(yr-wp)]	[m^3/(yr)]	[m^3/(yr-wp)]	[m^3/(yr-wp)]	[m^3/(yr-wp)]	[m^3/(yr-wp)]
0	8808.2	6.0537	0	0	0	6.0537	6.0537
50.988	8808.2	6.0537	6865.4	0.079027	0.079	5.9747	5.9747
1022.0	8956.2	6.1555	5680.3	0.065385	0.065	6.0901	6.0905
3003.8	10371	7.1278	6852.1	0.078874	0.079	7.0492	7.0488
10000	20125	13.8316	15062	0.17338	0.173	13.658	13.659
35200	51810	35.6082	51810	0.59639	0.596	35.012	35.012
74800	30951	21.2722	30951	0.35627	0.356	20.916	20.916
100000	8517.8	5.8542	8517.8	0.098048	0.098	5.7561	5.7562

Drip Shield Failure Time: 6294.607 years

 $\{q2\}$ calculated using q1 - q2

q4 generated by adding print statements to releaset

{q4} calculated by multiplying (q2' * flow multiplication factor * fmult * fow) where,

flow multiplication factor = 1.435932

fmult = 0.044721fow = 0.173205

Time [yr] $\{q2\}$ {q4} [m^3/(yr-wp)] [m^3/(yr-wp)] [m^3/(yr-wp)] 50.988 0.079027 1022.0 0 0.065385 0 3003.8 0.078874 0 10000 0.17338 0.0019285 0.001928 0.59639 0.0066334 0.006633

74800	0.35627	0	0.0039627	0.003963
100000	0.098048	0	0.0010905	0.001091

q5 is set equal to q4 after the waste package has filled. Since the bathtub model was used, the maximum volume of water in the waste package is determined by printing the volume to the screen.

 $vmax = 4.689 \text{ m}^3 \text{ (initial defects)}$

q5 generated by adding print statements to releaset

{q5} determined by calculating the waste package volume over time and comparing it to the maximum volume

The table shows a small difference between the calculated time when flow leaves the waste package compared to the results from the code. The times are close and the difference is most likely due to the error introduced in the hand calculations by using a constant value for q4 over each of the time intervals.

Time [yr]	q4 [m^3/(yr-wp)]	Change in waste package volume {initial defects}	volume in waste package {initial defects}	q5 [m^3/(yr-wp)] {initial defects}	{q5} [m^3/(yr-wp)] {initial defects}
6407.3	0.0012400	0	0	0	0
6559.6	0.0012831	0.1889	0.1889	0	0
6715.4	0.0012836	0.1999	0.3888	0	0
6875.0	0.0013009	0.2049	0.5937	0	0
7038.2	0.0013577	0.2123	0.8060	0	0
7205.3	0.0013583	0.2269	1.0329	0	0
7376.3	0.0013812	0.2323	1.2652	0	0
7551.3	0.0014364	0.2417	1.5069	0	0
7730.4	0.0014370	0.2573	1.7642	0	0
7913.7	0.0014810	0.2634	2.0276	0	0
8101.3	0.0015190	0.2778	2.3054	0	0
8293.3	0.0015193	0.2916	2.5970	0	0
8489.7	0.0016003	0.2984	2.8954	0	0
8690.8	0.0016053	0.3218	3.2172	0	0
8896.6	0.0016505	0.3304	3.5476	0	0
9107.2	0.0016946	0.3476	3.8952	0	0
9322.7	0.0017131	0.3652	4.2604	0	0
9543.3	0.0017876	0.3779	4.6383	0.0017876	0
9769.0		0.4035	{5.0418} 4.689 max	0.0017882	0.0017882

 $vmax = 0.28348 \text{ m}^3 \text{ (corrosive defects)}$

q5 generated by adding print statements to releaset

{q5} determined by calculating the waste package volume over time and comparing it to the

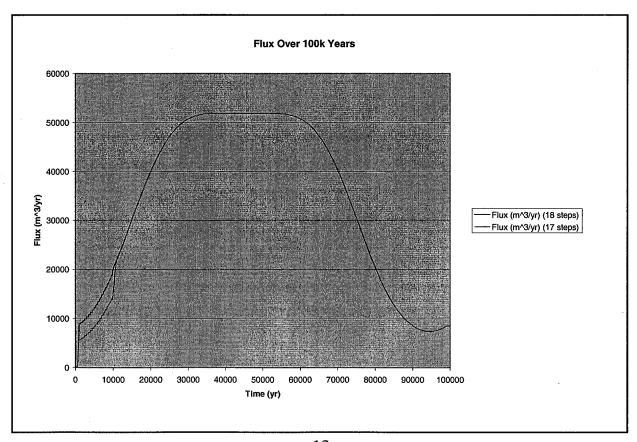
maximum volume

The calculated result compares to the information generated to the screen.

Time [yr]	q4 [m^3/(yr-wp)]	Change in waste package volume {corrosive defects}	volume in waste package {corrosive defects}	q5 [m/3/(yr-wp)] {corrosive defects}	{q5} [m^3/(yr-wp)] {corrosive defects}
67600	0.0056555	0	0	0	0
68500		5.08995	{5.08995} 0.28348 max	0.0054758	0.0054758

April 23, 2003 GADAMS:

Modified code module nfenv.f from tpa4.1j to align columns and column headers in reflux3.out. Executed the code for two test cases. In one test case, the drythick.dat file with 17 time steps was used which is its default in the tpa code. In the second test case, the drythick.dat file was modified to contain an initial parameter of 18 steps instead of the 17 steps for this parameter currently in the file. There are actually 18 rows of time data instead of 17. A plot of the amount of water that reaches the drift is shown below:



Test results are located on ZIP disk SN532E-VOL4:DISK1 in archive SPOCKHOMEtpabuild_studytpa41jmodrunTEST4-15-03.

May 20, 2003 GADAMS:

The TPA5.0d code was modified in two separate ways to identify the effect of natural backfill on the waste package temperature profile. The code modules exec.f, seismo2.f, and mechfail.f were modified to generate the static load height versus time and the drift height versus time. A test run was conducted over 10 realizations to generate an average drift height versus time and an average static load height versus time. A verification study was conducted on the modified code to verify that the inclusion of the two additional columns of static load height and drift height in seismo.rlt did not affect the other seismo results. In addition, hand calculations were conducted for static load height and drift height to verify the values generated at two specific times, 144.64 years and 730.86 years. The hand calculations are shown below:

```
Hand calculations to verify drift height and static load height.
Using SPOCK$HOMEtpabuild_studytpa50dmod5-14-03verificationtest2,
Drift Void Area (Ad) = 16.147547590502
Drift Radius (rd) = 2.75
Bulking Factor (bf) = 1.2915 (grid element 1)
                    = 1.48895 (grid element 2)
Maximum Drift Height (Hmax) = 2 * Ad + rd**2 * (bf-1)
                              pi * rd * (bf - 1)
Hmax1 = 2 * 16.1475475 + 2.75**2 * (1.2915 - 1)
         pi * 2.75 * (1.2915 - 1)
       = 13.699
 Hmax2 = 2 * 16.1475475 * 2.75**2 * (1.48895 - 1)
         pi 2.75 * (1.48895 - 1)
       = 8.5206
Drift Degradation Time (Tg) = 825.066 (grid element 1)
                            = 718.043 (grid element 2)
Drift Degradation Rate (g) = Hmax / Tg
 g1 = 13.699 / 825.066 = 0.01327
 g2 = 8.5206 / 718.043 = 0.00804
```

```
At time = 144.64
 drift height (h) = ho + g * delta time
   h1 = 2.75 + 0.01327 * 144.64 = 4.66937
   h2 = 2.75 + 0.00804 * 144.64 = 3.9124
 drip shield height (hds) = 2.521
 invert height (c) = 0.721
 static load height (hlh) = bf(h - rd) + 2(rd - Ad/(pi*rd)) - (hds - c)
   h1h1 = 1.2915 * (4.66937 - 2.75) + 2 * (2.75 - 16.14755/(pi * 2.75)) -
(2.521 + 0.721)
        = 0.99877
  h1h2 = 1.48895 * (3.9124 - 2.75) + 2 * (2.75 - 16.14755/(pi * 2.75)) -
(2.521 + 0.721)
        = 0.2506
          (below 0.5, the threshold, set to zero)
   hlhtotal = 0.75 * 0.99877 + 0.25 * 0 = 0.75
              (compares to static load height of 0.749153)
   htotal = 0.75 * 4.66937 + 0.25 * 3.9124 = 4.48
            (compares to drift height of 4.48021)
At time = 730.86,
  h1 = 2.75 + 0.01327 * 730.86 = 12.4485
  h2 = 2.75 + 0.00804 * 730.86 = 8.62611 (8.5206 is the maximum drift height)
 h1h1 = 1.2915 * (12.4485 - 2.75) + 2 * (2.75 - 16.14755/(pi * 2.75)) -
(2.521 + 0.721)
       = 11.045
  h1h2 = 1.48895 * (8.5206 - 2.75) + 2 * (2.75 - 16.14755/(pi * 2.75)) -
(2.521 + 0.721)
       = 7.112
  hlhtotal = 0.75 * 11.045 + 0.25 * 7.112 = 10.06
             (compares to static load height in seismo.rlt (subarea 10) of
  htotal = 0.75 * 12.4485 + 0.25 * 8.5206 = 11.47
           (compares to drift height in seismo.rlt (subarea 10) of 11.4669)
```

The second modification to the tpa5.0d code was to allow the code to use the static load height versus time and the drift height versus time in the form of an equivalent radius for natural backfill and an equivalent drift radius. In this case, the tpa5.0d code was used, but the NFENV.F module was modified to retrieve and interpolate the time variations of equivalent drift radius and equivalent natural backfill radius from file eqradius.dat placed within the data directory. Hand calculations were conducted to verify the temperature of the waste package at 128.32 years. The hand calculations are shown below:

The following hand calculation was used to verify the surface temperature calculation:

The time selected was 128.32 years, the calculations are as follows:

```
Gconv = 0.75 * 2 * pi * 0.9 * 6.1392
                                   -----= 27.98460296
       ln(2.75/1.579) + ln(2(3.448057513)/2(2.368379888))
Grad = 0.75 * 4 * 5.67e-8 * (273 + 166.43)**3
(1-0.87)/(0.87 * pi * 1.579*5.275) + 1 / (1.0 * pi * 1.579 * 5.275) + (1-0.63) / (0.63 * pi * 2.75 * 6.1392)
     = 262.4306922
Gcond = (1-0.75) * 2 * pi * 0.6 * 6.1392 / ln(5.5/1.579) = 4.636427912
Gcond(above) = (0.75 * 2 * pi * 6.1392)
            (1/0.27) * \ln(2(2.368379888) / (2.75 + 2(0.015))) + (1/20.77) *
ln((2.75 + 2(0.015)) / 2.75)
            = 14.65392906
Note: printed Qwp values to the screen: att 128.32 years, Qwp =
1926.123678299484
Twp = Qwp
                                              Trock
     Grad + Gconv + Gcond + Gcond(above)
   = 1926.123678299484
      _____
                                                                166.430
     262.4306922 + 27.98460296 + 4.636427912 + 14.65392906
   = 172.6492074
Using the NFENV.RLT file for test 1 in directory:
SPOCK$HOME/tpabuild_study/tpa50dmod5-15-03/run/test1,
at a time of 1.2832E+02 years, the value for tempwp is 1.7265E+02. This value
agrees with the
hand calculation above.
```

Note: in the calculations above, the calculation for gcond(above) or gcond_post in the code was modified to remove the effective thermal conductivity of the backfill from the numerator and to set the drip shield outer diameter to the sum of the inner diameter plus twice the drip shield thickness instead of the sum of the inner diameter and the drip shield thickness.

```
The original calculation is shown below:
```

The modified calculation is shown below:

```
gcond_post = 2.0d0 * pi * wpspace /
```

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```
& ( (dlog(bf_odia/(ds_idia + 2*dsthick)))/condbf +
& (dlog((ds_idia+ 2*dsthick)/ds_idia))/condds )
```

Test results and code are located on ZIP disk SN532E-VOL4:DISK 1 in archive:

SPOCKHOMEtpabuild_studytpa50dmod5-14-03 for the code and verification to generate the static load height and drift height versus time.

SPOCKHOMEtpabuild_studyTEST5-14-03 for test results over 10 realizations in which the static load height and drift height were generated.

SPOCKHOMEtpabuild_studymodifiedfiles50d5-14-03 for files modified to generate static load height and drift height versus time.

SPOCKHOMEtpabuild_studytpa50dmod5-15-03 for the code and verification for generating waste package temperature using the equivalent natural backfill radius and equivalent drift radius.

SPOCKHOMEtpabuild_studymodifiedfiles50d5-15-03 for files modified and added to use the equivalent natural backfill radius and equivalent drift radius.

June 4, 2003 GADAMS:

A modification was made to the tpa5.0d code to incorporate updates made to the thermal equations. The nfenv.f file was modified to incorporate three separate cases. Case 1 includes the waste package and no drip shield or backfill. Case 2 includes the waste package and drip shield but no backfill. And, Case 3 includes the waste package, drip shield and backfill. In addition, an update was made to the tpa.inp input file to include the emissivity of the backfill. This parameter was set to a constant value of 0.8. Two test cases were run to verify the modifications to the code against hand calculations. For test case 1, the backfill thickness was left at 0.0m. For test case 2, the backfill thickness was set to 0.5m. Therefore, test case 1 exercises Case 1 and Case 2 of the thermal equations and test case 2 exercises Case 1 and Case 3 of the thermal equations. The hand calculations are as follows:

```
Hand calculations to verify equations implemented for Thermal Model
```

For Case 1, the analysis was conducted at a time of 28.605 years and a temperature at the wall of 93.966 C.

For Case 2 and Case 3, the analysis was conducted at a time of 103.52 years and a temperature at the wall of 172.19 C.

```
BFThick[m] = \{0.5 \text{ for case } 3, 0.0 \text{ for case } 2\}
```

```
CircumFraction = 0.75
DiameterDSinner[m] = 2.75
DiameterRW[m] = 5.5
DiameterWP[m] = 1.579
DSThick[m] = 0.015
EmissDS = 0.63
EmissRW = 0.8
EmissWP = 0.87
EmissBF = 0.8 (Assumed value for this analysis - not currently in tpa.inp)
keff_nc[W/(m-C)] = 0.9
kfloor[W/(m-c) = 0.6]
kBF [W/(m-c)] = 0.27
pi = 3.14159
Stefan [W/(m^2k^4)] = 5.67e-8
wpspace[m] = 6.1392
Case 1
(Conduction through the floor/invert)
Gk1 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.6364
(Convection from the waste package to the rock wall)
Gc1 = 2 * 3.14159 * CircumFraction * WPSpace * keff_nc
       ln(DiameterRW / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(5.5 / 1.579)
     = 20.86
Gr1 = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
     ______
     (1 / (DiameterWP * EmissWP)) + ((1 - EmissRW) / (DiameterRW * EmissRW))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((93.966 + 273.15)**3)
       (1 / (1.579 * 0.87)) + ((1 - 0.8) / (5.5 * 0.8))
     = 162.3213102
       0.727945084 + 0.045454545
     = 209.880
```

```
Gtotal = Gk1 + Gc1 + Gr1
      = 4.6364 + 20.86 + 209.880
      = 235.3764
TempWP = (Qwp / Gtotal) + TempRW
      = (1388.8 / 235.3764) + 93.966
      = 99.866
The values calculated in Case 1 are comparable to the values in
thermalcase1-2.dat and nfenvcase1-2.rlt at 28.605 years.
The values calculated in Case 1 are comparable to the values in
thermalcase1-3.dat and nfenvcase1-3.rlt at 28.605 years.
Case 2
(Conduction through the floor/invert)
Gk2 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.6364
(Convection from the waste package to the drip shield)
Gc2pd = `2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterDSinner / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(2.75 / 1.579)
     = 46.93
(Convection from the drip shield to the wall rock)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                 = 2.75 + 2 * 0.015
                 = 2.78
Gc2dw = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterRW / DiameterDSouter)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(5.5 / 2.78)
     = 38.16
```

```
(Radiation from the waste package to the drip shield)
Gr2pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
     = 5.67e - 8 * 0.75 * 3.14159 * 6.1392 * 4 * ((172.19 + 273.15)**3)
       (1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 289.761523
       0.727945084 + 0.213564214
     = 307.763
(Radiation from the drip shield to the rock wall)
Gr2dw = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterDSouter * EmissDS)) + ((1 - EmissRW) / (DiameterRW *
EmissRW))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((172.19 + 273.15)**3)
       (1 / (2.78 * 0.63)) + ((1 - 0.8) / (5.5 * 0.8))
     = 289.761523
       0.570971794 + 0.045454545
     = 470.067
Gtotal = Gk2 +
             Gc2pd + Gr2pd Gc2dw + Gr2dw
      = 4.6364 +
                           1
                ______
                 46.93 + 307.763 38.16 + 470.067
      = 4.6364 +
                         1
                 _____
                0.00281934 + 0.001967625
      = 213.537
TempWP = (Qwp / Gtotal) + TempRW
      = (2227.2 / 213.537) + 172.19
      = 182.62
```

The values calculated for Case 2 are comparable to the values in nfenvcase1-2.rlt and thermalcase1-2.dat for 103.52 years.

```
Case 3
(Conduction through the floor/invert)
Gk3 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
                             ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.6364
(Convection from the waste package to the drip shield)
Gc3pd = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterDSinner / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(2.75 / 1.579)
     = 46.93
(Convection from the backfill to the drift wall)
DiameterBF[m] = DiameterDSinner + 2 * (DSThick + BFThick)
            = 2.75 + 2 * (0.015 + 0.5)
            = 3.78
Gc3bw = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterRW / DiameterBF)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(5.5 / 3.78)
     = 69.428
(Radiation from the waste package to the drip shield)
Gr3pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((172.19 + 273.15)**3)
       (1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 289.761523
       0.727945084 + 0.213564214
```

```
= 307.763
(Radiation from the backfill to the rock wall)
Gr3bw = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterBF * EmissBF)) + ((1 - EmissRW) / (DiameterRW *
EmissRW))
     = 5.67e - 8 * 0.75 * 3.14159 * 6.1392 * 4 * (172.19 + 273.15)**3)
       (1 / (3.78 * 0.8)) + ((1 - 0.8) / (5.5 * 0.8))
     = 289.761523
       0.330687831 + 0.045454545
     = 770.351
(Conduction through the backfill material)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                  = 2.75 + 2 * 0.015
                  = 2.78
Gbf3 = 2 * pi * WPSpace * (1 - CircumFraction) * kBF
      ln(DiameterBF / DiameterDSouter)
     = 2 * 3.14159 * 6.1392 * (1 - 0.75) * 0.27
      ln(3.78 / 2.78)
    = 8.474
Gtotal = Gk3 +
              Gc3pd + Gr3pd Gbf3 Gc3bw + Gr3bw
      = 4.6364 +
                                   1
                 _____
                                   1
                 ----- + ----- + ------
                 46.93 + 307.763 8.474 69.428 + 770.351
      = 4.6364 +
                 0.00282 + 0.118 + 0.00119
      = 12.832
TempWP = (Owp / Gtotal) + TempRW
      = (2227.2 / 12.832) + 172.19
```

= 345.76

The values calculated for Case 3 are comparable to the values in nfenvcase1-3.rlt and thermalcase1-3.dat at 103.52 years.

Test results and code are located on ZIP disk SN532E-VOL4:DISK 1 in archives: SPOCKHOMEtpabuild_studymodifiedfiles50d5-23-03.zip and SPOCKHOMEtpabuild_studytpa50dmod5-23-03.zip.

June 4, 2003 GADAMS:

A code modification was made to the tpa5.0d code that was identified under entry May 20, 2003 GADAMS tpa50dmod5-14-03. In the 5-14-03 version, only the static load height and drift height were generated. However, because of the effect of bulking factor, in order to calculate the equivalent area for backfill, the area of fallen rock also had to be generated to the seismo.rlt file.

This modified code is located on ZIP disk SN532E-VOL4:DISK 1 in archives: SPOCKHOMEtpabuild_studymodifiedfiles50d5-27-03.zip and SPOCKHOMEtpabuild_studytpa50dmod5-27-03.zip.

A second code modification was made to the tpa5.0d code that was identified under entry May 20, 2003 GADAMS tpa50dmod5-15-03. In the 5-15-03 version, a correction was made to the conductivity of the backfill term in which the effective thermal conductivity of the backfill was removed from the numerator. However, in order to generate a comparison to the equations used in the original TPA code, the correction was removed.

This modified code is located on ZIP disk SN532E-VOL4:DISK 1 in archives: SPOCKHOMEtpabuild_studymodifiedfiles50d5-27-03b.zip and SPOCKHOMEtpabuild_studytpa50dmod5-27-03b.zip.

June 5, 2003 GADAMS:

A series of tests were conducted in which the equivalent radius of the backfill and the equivalent radius of the drift were used to analyze waste package temperature. These tests are described below:

This test is designed to generate an average static load height versus time, an average drift height versus time, and an area of fallen rock versus time.

Test 1 uses 10 realizations. It uses version tpa50dmod5-27-03 of the tpa code.

Test 2 takes the equivalent radius for the backfill and the drift as an input file eqradius.dat. This file was generated using the area for backfill and the area of rock fallen from the drift in test cases a and b. It uses the arc length for backfill and the drift in test cases c and d.

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It uses version tpa50dmod5-27-03b of the tpa code. In test cases a and c, the thermal conductivity of the natural backfill is 0.27~W/(m-C) and in test cases b and d, the thermal conductivity of the natural backfill is 0.135~W/(m-C).

Test 3 uses the baseling tpa50d code and for test a runs the code with zero backfill thickness. For test b, the code is run with the maximum $(1.36\ m)$ of backfill.

Test 4 is a repeat of Test 1 except instead of running ten realizations, a single mean value realization is performed.

The seismo.rlt file from Test 4 was used for the Drift Height, Static Load Height, and Area of Fallen Rock versus time to generate an equivalent radius for the backfill and drift for the mean case.

The test results are located on ZIP disk SN532E-VOL4 DISK 1 in archive: SPOCKHOMEtpabuild_studyTEST5-27-03.

June 5, 2003 GADAMS:

A change was made to the tpa5.0d code to change the transition point at which chemistry values change. The current temperature transition point is tboil = 97C. The new value in the code is 80C. Only the portion of the code in which concentrations are assigned was modified to accommodate the temperature transition point.

The file drythick.dat was modified to contain 18 time steps.

The file tpa.inp was modified as follows:

```
constant
Indrift_Cl_PreTemperaturePeak[mol/L]
4.47E-2

-AND-
constant
Indrift_Cl_PostTemperaturePeak[mol/L]
4.48E-2
Were modified to:

constant
Indrift_Cl_PreTemperaturePeak[mol/L]
2.0

-AND-
```

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constant
Indrift_Cl_PostTemperaturePeak[mol/L]
2.0

A verification of the code change was conducted, the details of which follow:

A single run was performed to verify the code modification. The run was performed for 1 realization on subarea 1.

The first point of transition is as follows: (Extracted from NFENV.RLT) clwp time temprep tempwp relhumwp phwp 0.0000E+00 3.8571E+01 8.3700E+00 6.6500E-03 2.0000E+01 3.4170E-01 8.3900E+00 2 2.3102E+00 7.0903E+01 8.2948E+01 6.0762E-01 4.4700E-02

At a waste package temperature less than 80C, the new transition point, the chloride should come from multifbe.dat. The value in multifbe.dat is 6.65e-3 which corresponds the the value generated in the result file.

For this run, the critical relative humidity for aqueous corrosion is 0.4103218E+00. This parameter was taken from samplpar.res entry number 10.

At the second step above, the waste package temperature exceeds 80C, and the relative humidity exceeds the critical relative humidity. Therefore, the chloride concentration would be the value from tpa.inp as follows:

constant
Indrift_C1_PreTemperaturePeak[mol/L]
4.47E-2

As shown above, the value generated corresponds to the value in tpa.inp.

The second point of transition is as follows:

time temprep tempwp relhumwp phwp clwp 159 3.7221E+03 7.9627E+01 8.0165E+01 9.7843E-01 8.4000E+00 4.4800E-02 160 3.8116E+03 7.9044E+01 7.9576E+01 9.7856E-01 8.3700E+00 6.6500E-03

At this point of transition, after the peak temperature, the temperature of the waste package drops below 80C. Therefore, the value for chloride concentration

should come from file multifaf.dat. The value in this file is 6.65E-03 which corresponds to

the value generated by the code. On the previous line, with the time after the peak

and the temperature of the waste package above 80C and the relative humidity above the

critical relative humidity, the value for chloride concentration should be from the

tpa.inp file as follows:

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constant
Indrift_Cl_PostTemperaturePeak[mol/L]
4.48E-2

As shown above, the value generated corresponds to the value in tpa.inp.

This modified code is located on ZIP disk SN532E-VOL4:DISK 1 in archives: SPOCKHOMEtpabuild_studymodifiedfiles50d5-29-03.zip SPOCKHOMEtpabuild_studytpa50dmod5-29-03.zip.

June 5, 2003 GADAMS:

A test was conducted to evaluate edge effects within the repository using subarea 1 and subarea 2. The tpa50dmod5-29-03 version of the code was used in this study. The following is a summary of the tests conducted:

This test is conducted to evaluate the edge effects in the repository. Tests 1 to 3 are run on subarea 2 and tests 4 and 5 are run on subarea 1.

For all cases, the file drythick.dat is modified to contain 18 instead of seventeen time steps.

Test 1 is a mean base case run on subarea 2. The Test 1 subtest is run with the ThermalConductivityofYMRock[W/(m-K)] set to 1.56. The test is run with 50 realizations.

Test 2 is a mean TSW35 wet thermal conductivity test case on subarea 2. In this test, MassDensityofYMRock[kg/m^3] was set to 2540.0 SpecificHeatofYMRock[kg/m^3] was set to 900.0 ThermalConductivityofYMRock[W/(m-K)] was set to 2.02 The Test 2 subtest is run with the parameters above over 50 realizations.

Most 2 is a MCC24 rot thormal conductivity tost some with reduced both lo

Test 3 is a TSW34 wet thermal conductivity test case with reduced heat load on subarea 2.

Information in file drythick.dat is set to 0 for all steps.

In this test, MassDensityofYMRock[kg/m^3] was set to 2530.0

SpecificHeatofYMRock[kg/m^3] was set to 948.0

ThermalConductivityofYMRock[W/(m-K)] was set to 2.33

The Test 3 subtest is run with the parameters and files above over 50 realizations.

Test 4 is a mean base case run on subarea 1. The Test 4 subtest is run with the ThermalConductivityofYMRock[W/(m-K)] set to 1.56. The test is run with 50 realizations.

Test 5 is a TSW35 wet thermal conductivity test case on subarea 1 with reduced heat load.

In this test, MassDensityofYMRock[kg/m^3] was set to 2540.0 SpecificHeatofYMRock[kg/m^3] was set to 900.0

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 $Thermal Conductivity of YMRock [W/(m-K)] \ was \ set \ to \ 2.02$ The Test 5 subtest is run with the parameters and files above over 50 realizations.

Test 6 is a mean test case on subarea 1 with reduced heat load. The Test 6 subtest is run with 50 realizations.

The test results are located on ZIP disk SN532E-VOL4:DISK 1 in archive: SPOCKHOMEtpabuild_studyTEST5-28-03.

June 5, 2003 GADAMS

A change was made to the tpa5.0d version of the code to incorporate both the new thermal equations and the time varying values for equivalent backfill outer radius and equivalent drift radius. The code changes from version 5-27-03b and 5-23-03 were merged into this new code version.

This new code version is stored on ZIP disk SN532E-VOL4:DISK 1 in archives: SPOCKHOMEtpabuild_study/modifiedfiles50d6-2-03, SPOCKHOMEtpabuild_study/tpa50dmod6-2-03.

In addition, an error was found in the equation used to calculate the thermal conductivity of the backfill. The numerator of the equation contained the value 1 - the circumferential fraction not covered by the floor. It should have contained just the circumferential fraction not covered by the floor.

This new code version is stored on ZIP disk SN532E-VOL4:DISK 1 in archives: SPOCKHOMEtpabuild_study/modifiedfiles50d6-2-03b, SPOCKHOMEtpabuild_study/tpa50dmod6-2-03b.

June 5, 2003 GADAMS:

A series of tests were conducted to evaluate the effect of backfill on the temperature of the waste package. Four versions of the tpa code were used in this analysis: tpa5.0d, tpa50dmod5-27-03b, tpa50dmod6-2-03, and tpa50dmod6-2-03b. A description of these tests follows:

Tests 1 and 2 and 2b use version tpa50dmod6-2-03 and tests 3 and 4 use version tpa50dmod5-27-03b of the tpa code.

These tests use an equivalent radius for the backfill and drift based on the mean test case calculated from the area.

Test 1 was conducted using the egradius.dat file generated using area and

limited to the drift radius of 2.75m.

Test 2 is a repeat of Test 1; however, the thermal conductivity of the backfill was reduced in half to 0.135.

Test 2b is a repeat of Test 1; however, the thermal conductivity of the backfill was increased to 0.33.

Tests 3 and 4 repeat tests 1 and 2; however, the tpa code without the updated thermal equations is used.

Tests 5 and 6 use version tpa50dmod6-2-03b of the tpa code. In these tests, test 5 is run without backfill and test 6 is run with 1.36m of backfill.

Tests 7 and 8 are basecase tpa runs in which test 7 is run without backfill and test 8 is run with 1.36m of backfill.

In addition, a set of hand calculations was used to verify the results of the tests. These hand calculations are included as follows:

Hand calculations to verify equations implemented in updated heat transfer equations:

TEST1:

For Case 1, the analysis was conducted at a time of 28.605 years and a temperature at the wall of 87.281 C.

At 28.605 years, the backfill outer radius is 1.671895132 m.

The drift radius is 2.864358858 m.

For Case 3, the analysis was conducted at a time of 103.52 years and a temperature at the wall of 158.87 C.

At 103.52 years, the backfill outer radius is 2.248478084 m. The drift radius is 3.144202867 m.

A second run for test case 3 is run at a time of 200.98 years and a temperature at the wall of 142.04 C.

```
CircumFraction = 0.75
DiameterDSinner[m] = 2.75
DiameterRW[m] = 2 * 2.864358858 = 5.728717716 (@28.605 years),
                2 * 3.144202867 = 6.288405734 (@103.52 years),
                2 * 3.427945522 = 6.855891044 (@200.98 years)
DiameterBF[m] = 2 * 1.671895132 = 3.343790264 (@28.605 years),
                2 * 2.248478084 = 4.496956168 (@103.52 years),
                2 * 2.75
                                = 5.5
                                               (@200.98 years)
DiameterWP[m] = 1.579
DSThick[m] = 0.015
EmissDS = 0.63
EmissRW = 0.8
EmissWP = 0.87
EmissBF = 0.8 {Assumed value for this analysis - not currently in tpa.inp}
keff_nc[W/(m-C)] = 0.9
```

```
kfloor[W/(m-c) = 0.6]
kBF [W/(m-c)] = 0.27
pi = 3.14159
Stefan [W/(m^2k^4)] = 5.67e-8
wpspace[m] = 6.1392
Case 1
(Conduction through the floor/invert)
Gk1 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.64
(Convection from the waste package to the rock wall)
Gc1 = 2 * 3.14159 * CircumFraction * WPSpace * keff_nc
       ln(DiameterRW / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(5.728717716 / 1.579)
     = 20.20
Gr1 = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
     (1 / (DiameterWP * EmissWP)) + ((1 - EmissRW) / (DiameterRW * EmissRW))
     = 5.67e - 8 * 0.75 * 3.14159 * 6.1392 * 4 * ((87.281 + 273.15)**3)
       (1 / (1.579 * 0.87)) + ((1 - 0.8) / (5.728717716 * 0.8))
     = 153.6144293
       0.727945084 + 0.043639783
     = 199.09
Gtotal = Gk1 + Gc1 + Gr1
      = 4.64 + 20.20 + 199.09
      = 223.93
TempWP = (Qwp / Gtotal) + TempRW
      = (1388.8 / 223.93) + 87.281
      = 93.48
```

```
The values calculated in Case 1 are comparable to the values in
nfenv.rlt and thermal.dat at 28.605 years for test 1.
From nfenv.rlt and thermal.dat, the following values were present:
Gk1 = 4.6364E+00
Gc1 = 2.0204E+01
Gr1 = 1.9909E+02
Gtota1 = 2.2393E+02
TempWP = 9.3483E+01
Case 3
(Conduction through the floor/invert)
Gk3 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.64
(Convection from the waste package to the drip shield)
Gc3pd = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterDSinner / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(2.75 / 1.579)
     = 46.93
(Convection from the backfill to the drift wall)
Gc3bw = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterRW / DiameterBF)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(6.288405734 / 4.496956168)
     = 77.65
(Radiation from the waste package to the drip shield)
Gr3pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
```

= 5.67e - 8 * 0.75 * 3.14159 * 6.1392 * 4 * ((158.87 + 273.15)**3)

```
(1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 264.5313566
       0.727945084 + 0.213564214
     = 280.97
(Radiation from the backfill to the rock wall)
Gr3bw = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterBF * EmissBF)) + ((1 - EmissRW) / (DiameterRW *
EmissRW))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * (158.87 + 273.15)**3)
       (1 / (4.496956168 * 0.8)) + ((1 - 0.8) / (6.288405734 * 0.8))
     = 264.5313566
       0.277965796 + 0.039755704
     = 832.59
(Conduction through the backfill material)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                 = 2.75 + 2 * 0.015
                 = 2.78
Gbf3 = 2 * pi * WPSpace * CircumFraction * kBF
      ln(DiameterBF / DiameterDSouter)
    = 2 * 3.14159 * 6.1392 * 0.75 * 0.27
      ln(4.496956168 / 2.78)
    = 16.24
Gtotal = Gk3 +
                            1
              ----- + ---- + -----
              Gc3pd + Gr3pd Gbf3 Gc3bw + Gr3bw
      = 4.64
                                  1
                           1
                 ----- + ---- + ----
                = 4.64
                0.00304971 + 0.061576355 + 0.001098611
```

```
= 19.85
TempWP = (Qwp / Gtotal) + TempRW
      = (2227.2 / 19.85) + 158.87
      = 271.07
The values calculated in Case 3 are comparable to the values in
nfenv.rlt and thermal.dat at 103.52 years for test 1.
From nfenv.rlt and thermal.dat, the following values were present:
Gk3 = 4.6364E+00
Gc3pd = 4.6930E+01
Gr3pd = 2.8097E+02
Gbf3 = 1.6241E+01
Gc3bw = 7.7652E+01
Gr3bw = 8.3260E+02
Gtotal = 1.9852E+01
TempWP = 2.7106E+02
Case 3
A second run for test case 3 is run at a time of 200.98 years
and a temperature at the wall of 142.04 C.
(Conduction through the floor/invert)
Gk3 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.64
(Convection from the waste package to the drip shield)
Gc3pd = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterDSinner / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(2.75 / 1.579)
```

(Convection from the backfill to the drift wall)
Gc3bw = 2 * pi * CircumFraction * WPSpace * keff_nc

= 46.93

```
ln(DiameterRW / DiameterBF)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(6.855891044 / 5.5)
     = 118.16
(Radiation from the waste package to the drip shield)
Gr3pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((142.04 + 273.15)**3)
       (1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 234.8044135
       0.727945084 + 0.213564214
     = 249.39
(Radiation from the backfill to the rock wall)
Gr3bw = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
               ______
       (1 / (DiameterBF * EmissBF)) + ((1 - EmissRW) / (DiameterRW *
EmissRW))
     = 5.67e - 8 * 0.75 * 3.14159 * 6.1392 * 4 * (142.04 + 273.15)**3)
       (1 / (5.5 * 0.8)) + ((1 - 0.8) / (6.855891044 * 0.8))
     = 234.8044135
       0.227272727 + 0.03646499
     = 890.30
(Conduction through the backfill material)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                  = 2.75 + 2 * 0.015
                  = 2.78
Gbf3 = 2 * pi * WPSpace * CircumFraction * kBF
                 ________________
      ln(DiameterBF / DiameterDSouter)
     = 2 * 3.14159 * 6.1392 * 0.75 * 0.27
      ln(5.5 / 2.78)
    = 11.45
Gtotal = Gk3 +
                               1
```

```
1 1 1
             ----- + ---- + -----
             Gc3pd + Gr3pd Gbf3 Gc3bw + Gr3bw
      = 4.64
                                 1
                _____
                   1 1 1
                _____ + ____ + ____ + _____ + _____
                46.93 + 249.39 11.45 118.16 + 890.30
      = 4.64
                               1
                _____
                0.00337473 + 0.087336245 + 0.000991611
      = 15.54
TempWP = (Qwp / Gtotal) + TempRW
      = (1435.9 / 15.54) + 142.04
      = 234.44
The values calculated in Case 3 are comparable to the values in
nfenv.rlt and thermal.dat at 200.98 years for test 1.
From nfenv.rlt and thermal.dat, the following values were present:
Gk3 = 4.6364E+00
Gc3pd = 4.6930E+01
Gr3pd = 2.4940E+02
Gbf3 = 1.1448E+01
Gc3bw = 1.1816E+02
Gr3bw = 8.9032E+02
Gtotal = 1.5540E+01
TempWP = 2.3445E+02
TEST5:
For Case 2, a time of 200.98 years
and a temperature at the wall of 142.04 C.
CircumFraction = 0.75
DiameterDSinner[m] = 2.75
DiameterRW[m] = 5.5
DiameterBF[m] = 5.5
DiameterWP[m] = 1.579
DSThick[m] = 0.015
EmissDS = 0.63
EmissRW = 0.8
EmissWP = 0.87
EmissBF = 0.8 {Assumed value for this analysis - not currently in tpa.inp}
keff_nc[W/(m-C)] = 0.9
kfloor[W/(m-c) = 0.6]
kBF [W/(m-c)] = 0.27
pi = 3.14159
```

```
Stefan [W/(m^2k^4)] = 5.67e-8
wpspace[m] = 6.1392
Case 2
(Conduction through the floor/invert)
Gk2 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.6364
(Convection from the waste package to the drip shield)
Gc2pd = `2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterDSinner / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(2.75 / 1.579)
     = 46.93
(Convection from the drip shield to the wall rock)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                 = 2.75 + 2 * 0.015
                 = 2.78
Gc2dw = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterRW / DiameterDSouter)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(5.5 / 2.78)
     = 38.16
(Radiation from the waste package to the drip shield)
Gr2pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
     = 5.67e - 8 * 0.75 * 3.14159 * 6.1392 * 4 * ((142.04 + 273.15)**3)
       (1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 234.8044135
```

```
0.727945084 + 0.213564214
     = 249.39
(Radiation from the drip shield to the rock wall)
Gr2dw = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
        (1 / (DiameterDSouter * EmissDS)) + ((1 - EmissRW) / (DiameterRW *
EmissRW))
      = 5.67e - 8 * 0.75 * 3.14159 * 6.1392 * 4 * ((142.04 + 273.15)**3)
        (1 / (2.78 * 0.63)) + ((1 - 0.8) / (5.5 * 0.8))
     = 234.8044135
       0.570971794 + 0.045454545
     = 380.91
Gtotal = Gk2 +
              1 1
              Gc2pd + Gr2pd Gc2dw + Gr2dw
      = 4.6364 +
                   1
                 _____ + ______
                 46.93 + 249.39 38.16 + 380.91
      = 4.6364 +
                 0.00337473 + 0.002386236
      = 178.22
TempWP = (Qwp / Gtotal) + TempRW
      = (1435.9 / 178.22) + 142.04
      = 150.10
The values calculated in Case 2 are comparable to the values in
nfenv.rlt and thermal.dat at 200.98 years for test 5.
From nfenv.rlt and thermal.dat, the following values were present:
Gk2 = 4.6364E+00
Gc2pd = 4.6930E+01
Gr2pd = 2.4940E+02
Gc2dw = 3.8161E+01
Gr2dw = 3.8092E+02
Gtotal = 1.7822E+02
TempWP = 1.5010E+02
```

```
Percent contributions to flux for each of the terms:
Gk2 ==> (4.64 / 178.22) * 100 = 2.60%
Gc2pd + Gr2pd Gc2pd + Gr2pd Gc2dw + Gr2d2 = 0.974 / (46.93 + 249.39) / ((1 / (46.93 + 249.39)) + (1 / (38.16 + 380.91)))
Gc2pd + Gr2pd
                = 0.974 * 0.00337473 / (0.00337473 + 0.002386236)
                = 0.5706
      ______ (1 - 0.026) * ------ / (-----+ + -----
                Gc2dw + Gr2dw Gc2pd + Gr2pd Gc2dw + Gr2d2 = 0.974 / (38.16 + 380.91) / ((1 / (46.93 + 249.39)) + (1 / (38.16 + 380.91)))
Gc2dw + Gr2dw
                = 0.974 * 0.002386236 / (0.00337473 + 0.002386236)
                = 0.4034
Gc2pd ==> 0.5706 * Gc2pd
                  Gc2pd + Gr2pd
          = 0.5706 * 46.93 / (46.93 + 249.39)
          = 0.0904
Gr2pd ==> 0.5706 * Gr2pd
                  Gc2pd + Gr2pd
          = 0.5706 * 249.39 / (46.93 + 249.39)
          = 0.4802
Gc2dw ==> 0.4034 * Gc2dw
                  Gc2dw + Gr2dw
          = 0.4034 * 38.16 / (38.16 + 380.91)
          = 0.0367
Gr2dw ==> 0.4034 * Gr2dw
                 Gc2dw + Gr2dw
          = 0.4034 * 380.91 / (38.16 + 380.91)
          = 0.3667
Total conduction contribution to flux: 0.026
Total convection contribution to flux: 0.0904 + 0.0367 = 0.1271
Total radiation contribution to flux: 0.4802 + 0.3667 = 0.8469
TEST 6:
Test case 3 is run at a time of 200.98 years
and a temperature at the wall of 142.04 C.
CircumFraction = 0.75
DiameterDSinner[m] = 2.75
```

```
DiameterRW[m] =5.5
DiameterBF[m] = 5.5
DiameterWP[m] = 1.579
DSThick[m] = 0.015
EmissDS = 0.63
EmissRW = 0.8
EmissWP = 0.87
EmissBF = 0.8 (Assumed value for this analysis - not currently in tpa.inp)
keff_nc[W/(m-C)] = 0.9
kfloor[W/(m-c) = 0.6]
kBF [W/(m-c)] = 0.27
pi = 3.14159
Stefan [W/(m^2k^4)] = 5.67e-8
wpspace[m] = 6.1392
Case 3
(Conduction through the floor/invert)
Gk3 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
                             ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.64
(Convection from the waste package to the drip shield)
Gc3pd = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterDSinner / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(2.75 / 1.579)
     = 46.93
(Convection from the backfill to the drift wall)
Backfill out to the rock wall therefore no convection
(Radiation from the waste package to the drip shield)
Gr3pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
       (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((142.04 + 273.15)**3)
       (1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 234.8044135
```

```
0.727945084 + 0.213564214
     = 249.39
(Radiation from the backfill to the rock wall)
Backfill out to the rock wall therefore no radiation
(Conduction through the backfill material)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                  = 2.75 + 2 * 0.015
                  = 2.78
Gbf3 = 2 * pi * WPSpace * CircumFraction * kBF
      ln(DiameterBF / DiameterDSouter)
     = 2 * 3.14159 * 6.1392 * 0.75 * 0.27
      ln(5.5 / 2.78)
     = 11.45
Gtotal = Gk3 +
                  1 1
              Gc3pd + Gr3pd Gbf3
      = 4.64
                          1
                 _____ + ____
                 46.93 + 249.39 11.45
      = 4.64
                     1
                 0.00337473 + 0.087336245
      = 15.66
TempWP = (Qwp / Gtotal) + TempRW
      = (1435.9 / 15.66) + 142.04
      = 233.73
The values calculated in Case 3 are comparable to the values in
nfenv.rlt and thermal.dat at 200.98 years for test 6.
From nfenv.rlt and thermal.dat, the following values were present:
Gk3 = 4.6364E+00
Gc3pd = 4.6930E+01
Gr3pd = 2.4940E+02
Gbf3 = 1.1448E+01
Gtotal = 1.5659E+01
```

```
TempWP = 2.3374E+02
Percent contribution to flux for each of the terms:
Gk2 ==> (4.6364 / 15.659) = 0.2961
Gc3pd + Gr3pd Gc3pd + Gr3pd Gbf3
Gc3pd + Gr3pd
               = (0.7039 / (46.93 + 249.39)) / ((1 / (46.93 + 249.39)) +
                                              (1 / (11.45)))
               = 0.7039 * 0.00337473 / (0.00337473 + 0.087336245)
               = 0.0262
                                 1
---- ==> (1 - 0.2961) * ---- / (------+ ----)
                      Gbf3 Gc3pd + Gr3pd Gbf3
Gbf3
               = 0.7039 / (11.45) / ((1 / (46.93 + 249.39)) +
                                           (1 / (11.45))
               = 0.7039 * 0.087336245 / (0.00337473 + 0.087336245)
               = 0.6777
Total conduction contribution through the invert to flux: 0.2961
Total convection and radiation contribution to flux: 0.0262
Total conduction through the backfill contribution to flux: 0.6777
Case 1 at 28.605 years, temperature at the rock wall of 87.281 C
(Conduction through the floor/invert)
Gk1 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.64
(Convection from the waste package to the rock wall)
Gc1 = 2 * 3.14159 * CircumFraction * WPSpace * keff_nc
       ln(DiameterRW / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(5.5 / 1.579)
     = 20.86
Gr1 = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
     (1 / (DiameterWP * EmissWP)) + ((1 - EmissRW) / (DiameterRW * EmissRW))
     = 5.67e - 8 * 0.75 * 3.14159 * 6.1392 * 4 * ((87.281 + 273.15)**3)
       (1 / (1.579 * 0.87)) + ((1 - 0.8) / (5.5 * 0.8))
```

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These test results are included on ZIP disk SN532E-VOL4:DISK 2 in archive: SPOCKHOMEtpabuild_studyTEST6-2-03.

June 9, 2003 GADAMS:

A series of calculations were performed to evaluate the temperature of the drip shield using the new thermal equations with emplaced backfill. Calculations were performed on data from Test 5 and Test 6 contained in archive: APOCKHOME GADAMS June 9, 2003 SPOCKHOMEtpabuild_studyTEST6-2-03. Sample calculations at 1022 years showing the temperature of the drip shield with and without emplaced backfill follow:

Sample Calculations for Temperature of the Drip Shield at 1022 years

```
Test 5 (Case 2): TEST5:
```

For Case 2, a time of 1022 years and a temperature at the wall of 109.71 C.

CircumFraction = 0.75 DiameterDSinner[m] = 2.75 DiameterRW[m] = 5.5 DiameterBF[m] = 5.5

```
DiameterWP[m] = 1.579
DSThick[m] = 0.015
EmissDS = 0.63
EmissRW = 0.8
EmissWP = 0.87
EmissBF = 0.8 {Assumed value for this analysis - not currently in tpa.inp}
keff_nc[W/(m-C)] = 0.9
kfloor[W/(m-c) = 0.6]
kBF[W/(m-c)] = 0.27
pi = 3.14159
Stefan [W/(m^2k^4)] = 5.67e-8
wpspace[m] = 6.1392
Case 2
(Conduction through the floor/invert)
Gk2 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
   ln(DiameterRW / DiameterWP)
  = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
   ln(5.5 / 1.579)
  =4.6364
(Convection from the waste package to the drip shield)
Gc2pd = 2 * pi * CircumFraction * WPSpace * keff_nc
    ln(DiameterDSinner / DiameterWP)
   = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
    ln(2.75 / 1.579)
   =46.93
```

(Convection from the drip shield to the wall rock)

```
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
           = 2.75 + 2 * 0.015
          = 2.78
Gc2dw = 2 * pi * CircumFraction * WPSpace * keff_nc
    In(DiameterRW / DiameterDSouter)
   = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
    ln(5.5 / 2.78)
   = 38.16
(Radiation from the waste package to the drip shield)
Gr2pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
    (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner * EmissDS))
   = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((109.71 + 273.15)**3)
    (1/(1.579*0.87)) + ((1-0.63)/(2.75*0.63))
   = 184.1134798
    0.727945084 + 0.213564214
   = 195.55
(Radiation from the drip shield to the rock wall)
Gr2dw = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
    (1 / (DiameterDSouter * EmissDS)) + ((1 - EmissRW) / (DiameterRW * EmissRW))
   = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((109.71 + 273.15)**3)
    (1/(2.78*0.63)) + ((1-0.8)/(5.5*0.8))
   = 184.1134798
```

0.570971794 + 0.045454545

= 298.68

= 145.62

The values calculated in Case 2 are comparable to the values in nfenv.rlt and thermal.dat at 1022 years for test 5.

From nfenv.rlt and thermal.dat, the following values were present:

Gk2 = 4.6364E+00

Gc2pd = 4.6930E+01

Gr2pd = 1.9555E+02

Gc2dw = 3.8161E+01

Gr2dw = 2.9868E+02

Gtotal = 1.4562E+02

TempWP = 1.1299E+02

```
TempDS = ((Qwp - Gk2(TempWP - TempRW)) / (Gc2dw + Gr2dw)) + TempRW
= ((478.33 - 4.6364*(112.99-109.71)) / (38.16 + 298.68)) + 109.71
= 111.08
```

TEST 6:

Test case 3 is run at a time of 1022 years and a temperature at the wall of 109.71 C.

CircumFraction = 0.75

DiameterDSinner[m] = 2.75

DiameterRW[m] = 5.5

DiameterBF[m] = 5.5

DiameterWP[m] = 1.579

DSThick[m] = 0.015

EmissDS = 0.63

EmissRW = 0.8

EmissWP = 0.87

EmissBF = 0.8 {Assumed value for this analysis - not currently in tpa.inp}

keff nc[W/(m-C)] = 0.9

kfloor[W/(m-c) = 0.6]

kBF[W/(m-c)] = 0.27

pi = 3.14159

Stefan $[W/(m^2k^4)] = 5.67e-8$

wpspace[m] = 6.1392

(Conduction through the floor/invert)

Gk3 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor

ln(DiameterRW / DiameterWP)

= 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6

(Convection from the backfill to the drift wall)
Backfill out to the rock wall therefore no convection

(Radiation from the waste package to the drip shield)
Gr3pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3

(1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner * EmissDS))

= 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((109.71 + 273.15)**3)

(1/(1.579*0.87)) + ((1-0.63)/(2.75*0.63))

= 184.1134798

0.727945084 + 0.213564214

= 195.55

=46.93

(Radiation from the backfill to the rock wall)

Backfill out to the rock wall therefore no radiation

(Conduction through the backfill material)

DiameterDSouter[m] = DiameterDSinner + 2 * DSThick = 2.75 + 2 * 0.015

$$= 2.78$$

$$= 4.64 + 1$$

$$0.004124051 + 0.087336245$$

$$= 15.57$$

The values calculated in Case 3 are comparable to the values in nfenv.rlt and thermal.dat at 1022 years for test 6.

From nfenv.rlt and thermal.dat, the following values were present: Gk3 = 4.6364E+00

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Gc3pd = 4.6930E+01 Gr3pd = 1.9555E+02 Gbf3 = 1.1448E+01

Gtotal = 1.5569E+01

TempWP = 1.4043E+02

```
TempDS = -1 * (((Qwp - Gk3(TempWP - TempRW)) / (Gc3pd + Gr3pd)) - TempWP)
= -1 * (((478.33 - 4.6364*(140.43-109.71)) / (46.93 + 195.55)) - 140.43)
= 139.04
```

The temperature of the drip shield without emplaced backfill was 111.08 C at 1022 years and was 139.04 C at 1022 years with emplaced backfill.

June 11, 2003 GADAMS:

The hand calculations for drip shield temperature that were included in the previous entry (June 9, 2003 GADAMS) were incorporated into an Excel Spreadsheet for Test 5 and Test 6 also discussed in the previous entry. The spreadsheet is included in archive: Drift Degradation_In Drift.zip.

June 17, 2003 GADAMS:

A change was made to the nfenv module for tpa version 5.0d to analyze the effects of conduction through the backfill material along parallel paths. In one path, degradation of the drift was allowed, and in the other path, degradation was not allowed. The percentage of the drift allowed to degrade was specified in tpa.inp.

Two modifications were made to tpa.inp. constant EmissivityOfBackfill[-] 0.8

constant
CircumferentialFractionAllowedToDegrade[]
0.25

To analyze the portion of the drift allowed to degrade, the

CircumferentialFractionAllowedToDegrade[] parameter was modified as follows:

Scenario 1: 0.25 Scenario 2: 0.35 Scenario 3: 0.50

Scenario 4: 0.75 Scenario 5: 0.10

```
Hand calculations used to check the code modifications are as follows:
Hand calculations to verify equations implemented for Thermal Model
For Case 1, the analysis was conducted at a time of 28.605 years
and a temperature at the wall of 93.966 C.
For Case 3, the analysis was conducted at a series of scenarios.
Three different scenarios were analyzed.
The first scenario involved the following:
1) Time: 103.52 years, wall temperature of 158.87 C, 25% degradation fraction.
2) Time: 230.04 years, wall temperature of 139.57 C, 35% degradation fraction.
3) Time: 296.90 years, wall temperature of 135.16 C, 50% degradation fraction.
CircumFraction = 0.75
DiameterDSinner[m] = 2.75
DiameterRW[m] = 5.5
DiameterWP[m] = 1.579
DSThick[m] = 0.015
EmissDS = 0.63
EmissRW = 0.8
EmissWP = 0.87
EmissBF = 0.8 (Assumed value for this analysis - not currently in tpa.inp)
keff_nc[W/(m-C)] = 0.9
kfloor[W/(m-c) = 0.6]
kBF [W/(m-c)] = 0.27
pi = 3.14159
Stefan [W/(m^2k^4)] = 5.67e-8
wpspace[m] = 6.1392
DegradFraction = 0.25
Case 1
DriftHeight[m] = 3.10021
Delta Area of Drift = pi/2 * DiameterRW/2 * DriftHeight - pi/2 *
(DiameterRW/2)**2
                      = 3.14159 / 2 * 5.5 / 2 * 3.10021 - 3.14159 / 2 * (5.5 /
2) **2
                     = 1.512797322
Equivalent Diameter Drift = 2 * sqrt((Delta Area / DegradFraction + pi *
(DiameterRw / 2) **2) / pi)
                            = 2 * sgrt((1.512797322 / 0.25 + 3.14159 * (5.5 /
2) **2) / 3.14159)
                            = 2* 3.08036605
                            = 6.1607321
```

```
(Conduction through the floor/invert)
Gk1 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
    = 4.6364
(Convection from the waste package to the rock wall)
Gc1 = 2 * 3.14159 * CircumFraction * WPSpace * keff_nc
       ln(DiameterRW / DiameterWP)
     = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(6.1607321 / 1.579)
     = 19.12529
Gr1 = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
      ______
      (1 / (DiameterWP * EmissWP)) + ((1 - EmissRW) / (DiameterRW * EmissRW))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((87.281 + 273.15)**3)
        (1 / (1.579 * 0.87)) + ((1 - 0.8) / (6.1607321 * 0.8))
     = 153.6144293
       0.727945084 + 0.040579593
     = 199.882234
Gtotal = Gk1 + Gc1 + Gr1
      = 4.6364 + 19.12529 + 199.882234
      = 223.643924
TempWP = (Qwp / Gtotal) + TempRW
      = (1388.8 / 223.643924) + 87.281
      = 93.491
The values calculated in Case 1 are comparable to the values in
thermal.dat and nfenv.rlt at 28.605 years.
Values retrieved:
Gk1: 4.6364E+00
Gc1: 1.9125E+01
Gr1: 1.9988E+02
Gtotal: 2.2364E+02
TempWP: 9.3491E+01
```

```
Case 3, Scenario 1
Time: 103.52 years, wall temperature of 158.87 C, 25% degradation fraction.
DriftHeight[m] = 4.01737
Area of Fallen Rock[m^2] = 7.3597
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                  = 2.75 + 2 * 0.015
Delta Area of Drift = pi/2 * DiameterRW/2 * DriftHeight - pi/2 *
(DiameterRW/2) **2
                   = 3.14159 / 2 * 5.5 / 2 * 4.01737 - 3.14159 / 2 * (5.5 /
2) * * 2
                   = 5.474640763
Equivalent Diameter Drift = 2 * sqrt((Delta Area / DegradFraction + pi *
(DiameterRw / 2)**2) / pi)
                         = 2 * sqrt((5.474640763 / 0.25 + 3.14159 * (5.5 /
2) * * 2) / 3.14159)
                         = 2* 3.812221793
                         = 7.624443586
First calculate the equivalent radius of the backfill assuming that section b
of the drift
has not reached the maximum diameter of backfill.
Equivalent Diameter BF = 2 * sqrt((area fallen / CircumFraction + pi *
(DiameterDSouter / 2)**2) / pi)
                      = 2 * sqrt((7.3597 / 0.75 + 3.14159 * (2.78 / 2)**2) /
3.14159)
                      = 2 * 2.24847867
                      = 4.496957341
Since this diameter does not exceed 5.5m, the calculation above is valid as
the backfill outer diameter
for both section a (allowed to degrade) and section b (not allowed to degrade)
(Conduction through the floor/invert)
Gk3 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
     ln(DiameterRW / DiameterWP)
   = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
     ln(5.5 / 1.579)
   = 4.6364
(Convection from the waste package to the drip shield)
Gc3pd = 2 * pi * CircumFraction * WPSpace * keff_nc
       ln(DiameterDSinner / DiameterWP)
```

```
= 2 * 3.14159 * 0.75 * 6.1392 * 0.9
       ln(2.75 / 1.579)
     = 46.93
(Convection from the backfill to the drift wall)
Gc3bw == ignore for this scenario (conduction through the backfill dominates)
(Radiation from the waste package to the drip shield)
Gr3pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
            (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((158.87 + 273.15)**3)
        (1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 264.5313566
       0.727945084 + 0.213564214
      = 280.9652089
(Radiation from the backfill to the rock wall)
Gr3bw = ignore for this scenario (conduction through the backfill dominates)
(Conduction through the backfill material)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                   = 2.75 + 2 * 0.015
                   = 2.78
Gbf3_A = 2 * pi * WPSpace * DegradFraction * kBF
      ln(DiameterBF / DiameterDSouter)
     = 2 * 3.14159 * 6.1392 * 0.25 * 0.27
      ln(4.496957341 / 2.78)
     = 5.413710678
Gbf3_B = 2 * pi * WPSpace * (CircumFraction - DegradFraction) * kBF
      ln(DiameterBF / DiameterDSouter)
     = 2 * 3.14159 * 6.1392 * (0.75 - 0.25) * 0.27
      ln(4.496957341 / 2.78)
    = 10.82742136
Gtotal = Gk3 +
```

```
Gc3pd + Gr3pd Gbf3_A + Gbf3_B
      = 4.6364 +
                _____ + ____ + _____
                46.93 + 280.9652 5.413710678 + 10.82742136
      = 4.6364 +
                        1
                0.0030498 + 0.061572
      = 20.111
TempWP = (Qwp / Gtotal) + TempRW
      = (2227.2 / 20.111) + 158.87
      = 269.615
The values calculated for Case 3, scenario 1 are comparable to the values
in nfenv.rlt and thermal.dat at 103.52 years.
Values retrieved:
Gk3: 4.6364E+00
Gc3pd: 4.6930E+01
Gr3pd: 2.8097E+02
Gbf3_A: 5.4137E+00
Gbf3_B: 1.0827E+01
Gtotal: 2.0111E+01
TempWP: 2.6962E+02
//// Case 3, Scenario 2 ////
Time: 230.04 years, wall temperature of 139.57 C, 35% degradation fraction.
DriftHeight[m] = 5.56639
Area of Fallen Rock[m^2] = 16.355
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                 = 2.75 + 2 * 0.015
                 = 2.78
Delta Area of Drift = pi/2 * DiameterRW/2 * DriftHeight - pi/2 *
(DiameterRW/2)**2
                  = 3.14159 / 2 * 5.5 / 2 * 5.56639 - 3.14159 / 2 * (5.5 /
2)**2
                  = 12.16592116
Equivalent Diameter Drift = 2 * sqrt((Delta Area / DegradFraction + pi *
(DiameterRw / 2)**2) / pi)
                        = 2 * sqrt((12.16592116 / 0.35 + 3.14159 * (5.5 /
2) * * 2) / 3.14159)
                        = 2 * 4.315888007
```

= 8.631776014

```
First calculate the equivalent radius of the backfill assuming that section b
of the drift
has not reached the maximum diameter of backfill.
Equivalent Diameter BF = 2 * sqrt((area fallen / CircumFraction + pi *
(DiameterDSouter / 2)**2) / pi)
= 2 * sqrt((16.355 / 0.75 + 3.14159 * (2.78 / 2)**2) /
3.14159)
                        = 2 * 2.978822494
                        = 5.957644987
Since this diameter exceeds 5.5m, the calculation above is invalid. Section b
has already reached its
maximum diameter of 5.5m.
Area of Section B = (pi * (Diameter BF B / 2)**2 - pi * (Diameter DSouter / 2)**2) * (CircumFraction - DegradFraction)
                   = (3.14159 * (5.5 / 2)**2 - 3.14159 * (2.78 / 2)**2) * (0.75)
-0.35)
                   = 7.075363336
Equivalent Diameter B = 5.5
Equivalent Diameter A = 2 * sqrt(((Area Fallen - Area Section B) /
DegradFraction + pi * (DiameterDSouter / 2)**2) / pi)
= 2 * sqrt(((16.355 - 7.075363336) / 0.35 + 3.14159 *
(2.78 / 2)**2) / 3.14159)
                       = 2 * 3.220486913
                       = 6.440973826
(Conduction through the floor/invert)
Gk3 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
      ln(DiameterRW / DiameterWP)
    = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
      ln(5.5 / 1.579)
    = 4.6364
(Convection from the waste package to the drip shield)
Gc3pd = 2 * pi * CircumFraction * WPSpace * keff_nc
            _____
        ln(DiameterDSinner / DiameterWP)
      = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
        ln(2.75 / 1.579)
      = 46.93
(Convection from the backfill to the drift wall)
Gc3bw == ignore for this scenario (conduction through the backfill dominates)
(Radiation from the waste package to the drip shield)
```

```
Gr3pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
        (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
     = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((139.57 + 273.15)**3)
        (1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 230.6386811
       0.727945084 + 0.213564214
     = 244.9669712
(Radiation from the backfill to the rock wall)
Gr3bw = ignore for this scenario (conduction through the backfill dominates)
(Conduction through the backfill material)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                  = 2.75 + 2 * 0.015
                  = 2.78
Gbf3_A = 2 * pi * WPSpace * DegradFraction * kBF
      ln(DiameterBF / DiameterDSouter)
     = 2 * 3.14159 * 6.1392 * 0.35 * 0.27
      ln(6.440973826 / 2.78)
     = 4.338359328
Gbf3_B = 2 * pi * WPSpace * (CircumFraction - DegradFraction) * kBF
      ln(DiameterBF / DiameterDSouter)
    = 2 * 3.14159 * 6.1392 * (0.75 - 0.35) * 0.27
      ln(5.5 / 2.78)
    = 6.105784505
Gtotal = Gk3 +
              ______ + _____
              Gc3pd + Gr3pd Gbf3_A + Gbf3_B
      = 4.6364 +
                 46.93 + 244.9669712 4.338359328 + 6.105784505
      = 4.6364 +
                            1
```

```
0.003425866 + 0.095747437
      = 14.720
TempWP = (Qwp / Gtotal) + TempRW
= (1332.2 / 14.720) + 139.57
      = 230.073
The values calculated for Case 3, scenario 2 are comparable to the values
in nfenv.rlt and thermal.dat at 230.04 years.
Values retrieved:
Gk3: 4.6364E+00
Gc3pd: 4.6930E+01
Gr3pd: 2.4496E+02
Gbf3_A: 4.3384E+00
Gbf3 B: 6.1058E+00
Gtotal: 1.4720E+01
TempWP: 2.3007E+02
Case 3, Scenario 3
Time: 296.90 years, wall temperature of 135.16 C, 50% degradation fraction.
DriftHeight[m] = 6.47333
Area of Fallen Rock[m^2] = 21.6217
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                  = 2.75 + 2 * 0.015
                  = 2.78
Delta Area of Drift = pi/2 * DiameterRW/2 * DriftHeight - pi/2 *
(DiameterRW/2)**2
                   = 3.14159 / 2 * 5.5 / 2 * 6.47333 - 3.14159 / 2 * (5.5 /
2)**2
                   = 16.08361741
Equivalent Diameter Drift = 2 * sqrt((Delta Area / DegradFraction + pi *
(DiameterRw / 2) **2) / pi)
                         = 2 * sqrt((16.08361741 / 0.50 + 3.14159 * (5.5 /
2) **2) / 3.14159)
                         = 2 * 4.21920150
                         = 8.438402100
First calculate the equivalent radius of the backfill assuming that section b
of the drift
has not reached the maximum diameter of backfill.
Equivalent Diameter BF = 2 * sqrt((area fallen / CircumFraction + pi *
(DiameterDSouter / 2) **2) / pi)
```

```
= 2 * sqrt((21.6217 / 0.75 + 3.14159 * (2.78 / 2)**2) /
3.14159)
                       = 2 * 3.332962982
                       = 6.665925964
Since this diameter exceeds 5.5m, the calculation above is invalid. Section b
has already reached its
maximum diameter of 5.5m.
Area of Section B = (pi * (Diameter BF B / 2)**2 - pi * (DiameterDSouter /
2) **2) * (CircumFraction - DegradFraction)
                  = (3.14159 \times (5.5 / 2)**2 - 3.14159 \times (2.78 / 2)**2) \times (0.75)
-0.50)
                  = 4.422102085
Equivalent Diameter B = 5.5
Equivalent Diameter A = 2 * sqrt(((Area Fallen - Area Section B) /
DegradFraction + pi * (DiameterDSouter / 2)**2) / pi)
                      = 2 * sqrt(((21.6217 - 4.422\overline{102085}) / 0.50 + 3.14159 *
(2.78 / 2)**2) / 3.14159)
                      = 2 * 3.589110386
                      = 7.178220772
(Conduction through the floor/invert)
Gk3 = 2 * pi * WPSpace * (1 - CircumFraction) * kfloor
      ln(DiameterRW / DiameterWP)
    = 2 * 3.14159 * 6.1392 * (1.0 - 0.75) * 0.6
      ln(5.5 / 1.579)
    = 4.6364
(Convection from the waste package to the drip shield)
Gc3pd = 2 * pi * CircumFraction * WPSpace * keff_nc
        ln(DiameterDSinner / DiameterWP)
      = 2 * 3.14159 * 0.75 * 6.1392 * 0.9
        ln(2.75 / 1.579)
      = 46.93
(Convection from the backfill to the drift wall)
Gc3bw == ignore for this scenario (conduction through the backfill dominates)
(Radiation from the waste package to the drip shield)
Gr3pd = Stefan * CircumFraction * pi * WPSpace * 4 * TempRW**3
        (1 / (DiameterWP * EmissWP)) + ((1 - EmissDS) / (DiameterDSinner *
EmissDS))
      = 5.67e-8 * 0.75 * 3.14159 * 6.1392 * 4 * ((135.16 + 273.15)**3)
```

```
(1 / (1.579 * 0.87)) + ((1 - 0.63) / (2.75 * 0.63))
     = 223.3241299
       0.727945084 + 0.213564214
     = 237.1980079
(Radiation from the backfill to the rock wall)
Gr3bw = ignore for this scenario (conduction through the backfill dominates)
(Conduction through the backfill material)
DiameterDSouter[m] = DiameterDSinner + 2 * DSThick
                  = 2.75 + 2 * 0.015
                  = 2.78
Gbf3_A = 2 * pi * WPSpace * DegradFraction * kBF
      ln(DiameterBF / DiameterDSouter)
    = 2 * 3.14159 * 6.1392 * 0.50 * 0.27
      ln(7.178220772 / 2.78)
    = 5.489611963
Gbf3_B = 2 * pi * WPSpace * (CircumFraction - DegradFraction) * kBF
      ln(DiameterBF / DiameterDSouter)
    = 2 * 3.14159 * 6.1392 * (0.75 - 0.50) * 0.27
      ln(5.5 / 2.78)
    = 3.816115317
Gtotal = Gk3 +
               _____ + _____
              Gc3pd + Gr3pd Gbf3_A + Gbf3_B
      = 4.6364 +
                 -----+ -------
                 46.93 + 237.1980079 5.489611963 + 3.816115317
      = 4.6364 +
                 0.003519540 + 0.107460704
      = 13.647
```

TempWP = (Qwp / Gtotal) + TempRW

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```
= (1152.5 / 13.647) + 135.16
= 219.61
```

The values calculated for Case 3, scenario 3 are comparable to the values in nfenv.rlt and thermal.dat at 296.90 years.

Values retrieved: Gk3: 4.6364E+00 Gc3pd: 4.6930E+01 Gr3pd: 2.3720E+02 Gbf3_A: 5.4896E+00 Gbf3_B: 3.8161E+00 Gtotal: 1.3647E+01 TempWP: 2.1961E+02

The code was built and tested on machine spock. The code and test results are stored on ZIP disk: SN532E-VOL4:DISK2 in archives:

SPOCKHOMEtpabuild_studymodifiedfiles6-16-03 SPOCKHOMEtpabuild_studytpa50dmod6-16-03

June 20, 2003 GADAMS:

A series of two tests was conducted using version tpa50dmod6-16-03 of the tpa code. These tests were designed to approximate the case where the degradation portion of the drift is limited to the original radius of the drift. These tests were mean value cases and the only difference in the tpa.inp file was the value for CircumferentialFractionAllowedToDegrade[-]. For test 1, the value was set to 0.005 and for test 2, the value was set to 0.0001.

The test results are stored on ZIP disk: SN532E-VOL4:DISK2 in archive: SPOCKHOMEtpabuild_studyTEST6-17-03.zip.

October 1, 2003 GADAMS:

Tests involving drift degradation that were previously conducted using version tpa50d of the tpa code were repeated with version tpa50p. Differences from previous tests are as follows:

- 1) Drift degradation was set to occur after the operational period.
- 2) The distance into the rock wall was incorporated into the analysis. In this case, 0m is the drift wall, 1m is one meter into the rock wall, etc.

The test results are stored on ZIP disk: SN532E-VOL4:DISK3 in archive: SPOCKHOMEtpabuild_tef.zip.

October 21, 2003 GADAMS:

Updates to the drift degradation work were performed to include the following:

1) Hand calculations were updated to include emplaced backfill for case 3.

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2) An evaluation of the linearized versus the fully iterative solution for waste package temperature was included (both test runs and hand calculations).

The test results are stored on ZIP disk: SN532E-VOL4-DISK3 in archive: SPOCKHOMEtpabuild_teftef10-2-03.zip.

October 23, 2003 GADAMS:

Evaluated drift degradation at a point 5m into the rock wall using reduced heat load files (burnup.dat). The files were generated previously and contained in archive SPOCKHOMEtpabuild_studyTEST5-28-03 under entry June 5, 2003 GADAMS.

The test results are stored on ZIP disk: SN532E-VOL4:DISK3 in archive: SPOCKHOMEtpabuild_teftef10-22-03.zip.

October 27, 2003 GADAMS:

Evaluated waste package and drip shield temperatures at four different values (0.33 W/m-K, 0.27 W/m-K, 0.203 W/m-K, and 0.135 W/m-K) for the thermal conductivity of natural backfill. Evaluated these temperatures from calculations using a point at the drift wall and at a point 5m into the drift wall. In addition, the Thermal Effects Report.xls figure 3-7 and 3-8 plots were updated to display the drift wall temperatures for a thermal conductivity value of 0.27 W/m-K.

The test results are stored on ZIP disk: SN532E-VOL4:DISK3 in archive: SPOCKHOMEtpabuild_teftef10-27-03.zip.

October 31, 2003 GADAMS:

Conducted a mean case run using tpa version 5.0r to generate information for the time, temperature and flow of water into the repository.

The test results are stored on ZIP disk: SN532E-VOL4:DISK3 in archive: APOCKHOME GADAMS 10-31-2003 SPOCKHOMEtpabuild_studytest10-31-03.zip.

November 10, 2003 GADAMS:

Added the capability to retrieve rock temperatures from an external file and performed a set of test runs for the case of natural drift degradation with backfill and no backfill. Calculations were performed from a distance 5m into the rock. The version of the code modified to implement this change was SPOCKHOMEtpabuild_teftpa50pmod. The new version with this change was designated SPOCKHOMEtpabuild_teftpa50pdrift. The nfenv.f file was modified to incorporate this change.

The modified code and test results are stored on ZIP disk: SN532E-VOL4:DISK3 in archive:

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SPOCKHOMEtpabuild_teftpa50pdrift.zip.

November 13, 2003 GADAMS:

Performed a series of tests for emplaced backfill, early degradation, and east end using the tpa50pdrift version of the tpa code. Plots for the mountain scale conduction model and the tef model were made for these three cases.

The test results are stored on ZIP disk: SN532E-VOL4:DISK3 in archive SPOCKHOMEtpabuild_teftef11-13-03.zip.

Entries into Scientific Notebook #532E-Vol4 for pages ___\ - __\ have been made by George Adams 8/24/04.

No original text entered into this Scientific Notebook has been removed.

Dung Q Relson 8/24/04.

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

Dorden Wittingen 9/21/2004

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 532E

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File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Media contains: data files for in-drift thermal radiation and forced ventilation model to develop an interface model